



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 05:11 AM EDT

PDB ID : 9P76 / pdb_00009p76
EMDB ID : EMD-71333
Title : In situ human eEF1A-A/T-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.83 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

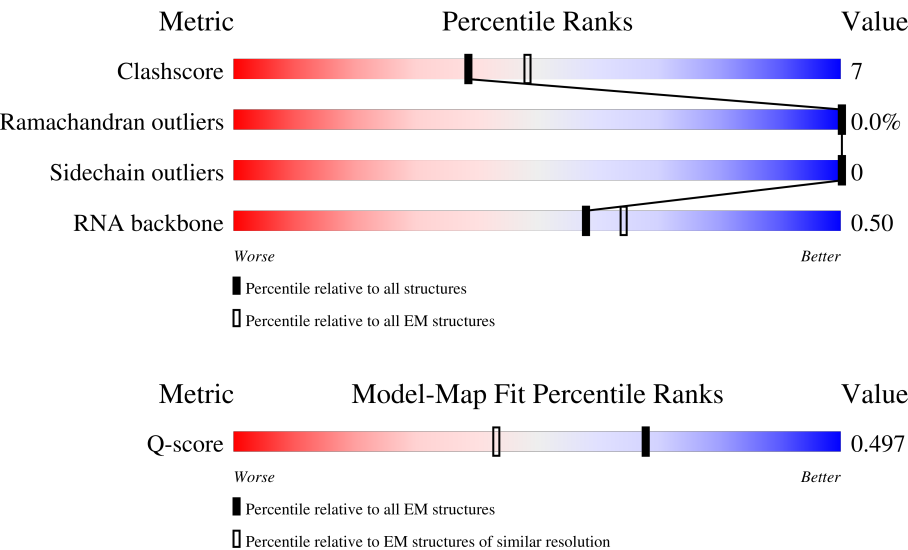
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



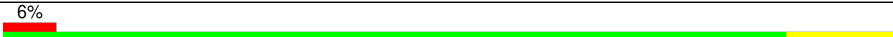
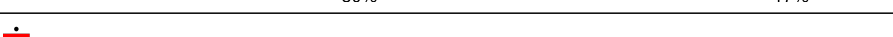
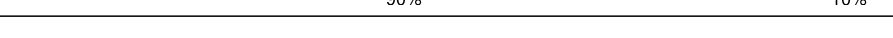
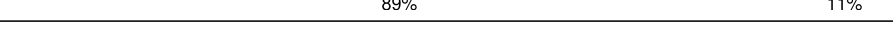
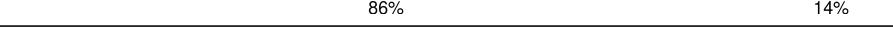
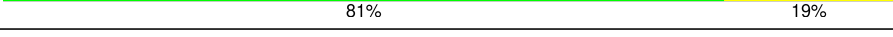
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CI	31	6% 71% 29%
2	Pt	74	54% 42%
3	CF	441	72% 28%

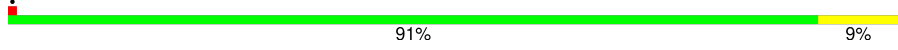
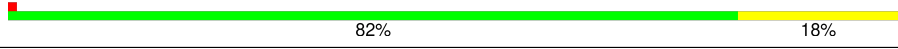
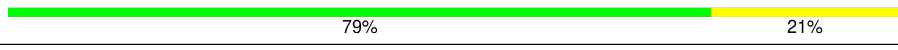
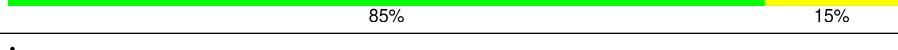
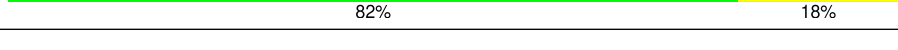
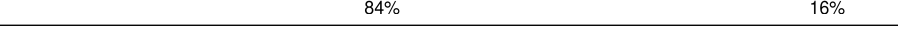
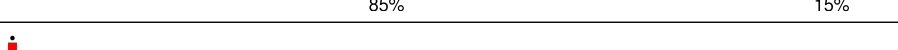
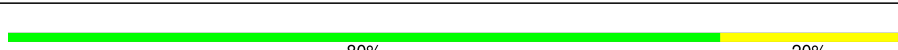
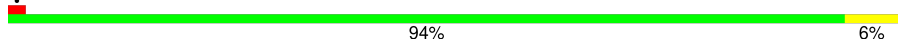
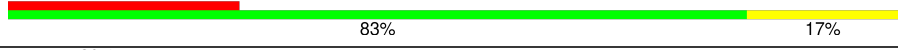
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Mol	Chain	Length	Quality of chain
4	AT	76	
5	L5	3655	
6	L7	120	
7	L8	156	
8	LA	248	
9	LB	402	
10	LC	368	
11	LD	293	
12	LE	250	
13	LF	225	
14	LG	241	
15	LH	190	
16	LI	213	
17	LJ	176	
18	LL	210	
19	LM	139	
20	LN	203	
21	LO	201	
22	LP	153	
23	LQ	187	
24	LR	187	
25	LS	175	
26	LT	159	
27	LU	101	
28	LV	131	

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Mol	Chain	Length	Quality of chain
29	LW	124	
30	LX	120	
31	LY	134	
32	LZ	135	
33	La	147	
34	Lb	121	
35	Lc	98	
36	Ld	107	
37	Le	128	
38	Lf	109	
39	Lg	114	
40	Lh	122	
41	Li	102	
42	Lj	86	
43	Lk	69	
44	Ll	50	
45	Lm	52	
46	Ln	24	
47	Lo	105	
48	Lp	91	
49	Lr	125	
50	Ls	196	
51	Lt	157	
52	SD	227	
53	SF	189	

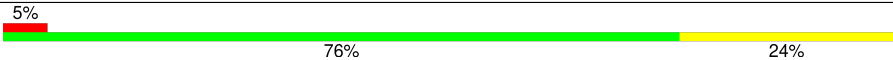
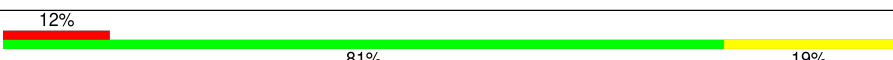
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Mol	Chain	Length	Quality of chain
54	SK	98	
55	SM	122	
56	SP	121	
57	SQ	144	
58	SR	135	
59	SS	145	
60	ST	143	
61	SU	104	
62	SZ	75	
63	Sc	64	
64	Sd	55	
65	Sf	67	
66	Sg	313	
67	SA	221	
68	SB	214	
69	SC	220	
70	SE	262	
71	SG	237	
72	SH	189	
73	SI	206	
74	SJ	185	
75	SL	153	
76	SN	150	
77	SO	137	
78	SV	83	

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Mol	Chain	Length	Quality of chain
79	SW	129	 81% 19%
80	SX	141	 82% 18%
81	SY	131	 5% 76% 24%
82	Sa	102	 83% 17%
83	Sb	83	 82% 18%
84	Se	58	 12% 81% 19%
85	S2	1740	 49% 42% 9%

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 223377 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

- Molecule 2 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

- Molecule 3 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
3	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 4 is a RNA chain called AT site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 7 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 8 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 9 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 10 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 11 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 12 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 13 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 14 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 15 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 16 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 17 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 18 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 19 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 20 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 21 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 22 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 23 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 26 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 27 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 30 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 31 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 32 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 33 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 34 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 35 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 36 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 37 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 38 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 39 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 40 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 41 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 42 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 43 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 44 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 45 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 46 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 47 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 48 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 49 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 50 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 51 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

- Molecule 52 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 54 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 55 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 56 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 57 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 58 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 59 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 60 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 61 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 62 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 63 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 64 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 65 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 67 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 68 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 69 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 70 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 71 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 72 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 73 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 74 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 75 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 76 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 77 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 78 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 79 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 80 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 82 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 83 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 84 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 85 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

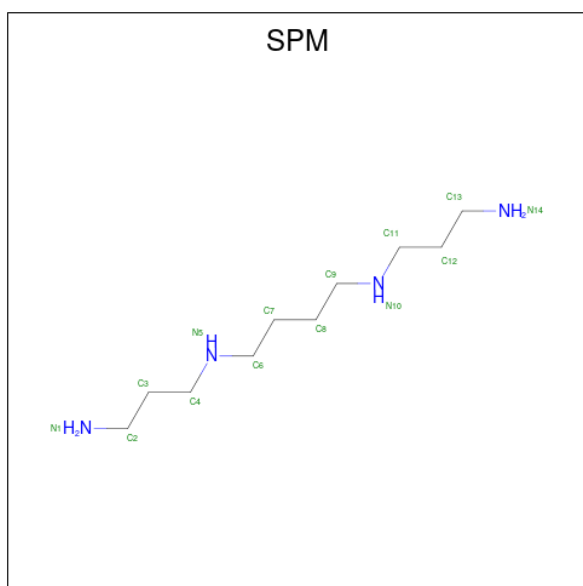
Mol	Chain	Residues	Atoms		AltConf
86	L5	178	Total	Mg	0
			178	178	
86	L7	3	Total	Mg	0
			3	3	
86	L8	4	Total	Mg	0
			4	4	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	SS	1	Total	Mg	0
			1	1	
86	SG	1	Total	Mg	0
			1	1	
86	S2	26	Total	Mg	0
			26	26	

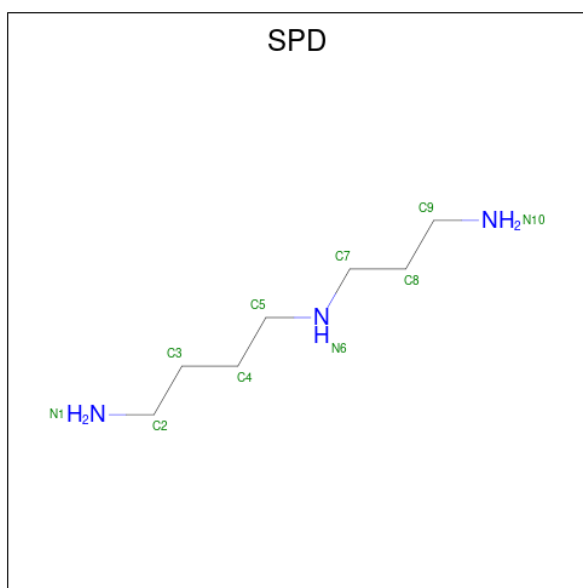
- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).

Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	LN	1	Total	C	N	0
			10	7	3	

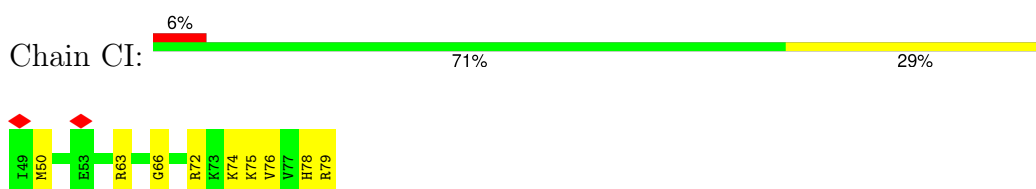
- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
89	Lg	1	Total 1	Zn 1	0
89	Lj	1	Total 1	Zn 1	0
89	Lm	1	Total 1	Zn 1	0
89	Lo	1	Total 1	Zn 1	0
89	Lp	1	Total 1	Zn 1	0
89	Sa	1	Total 1	Zn 1	0

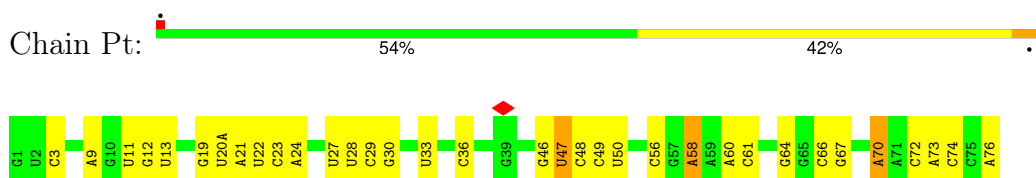
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

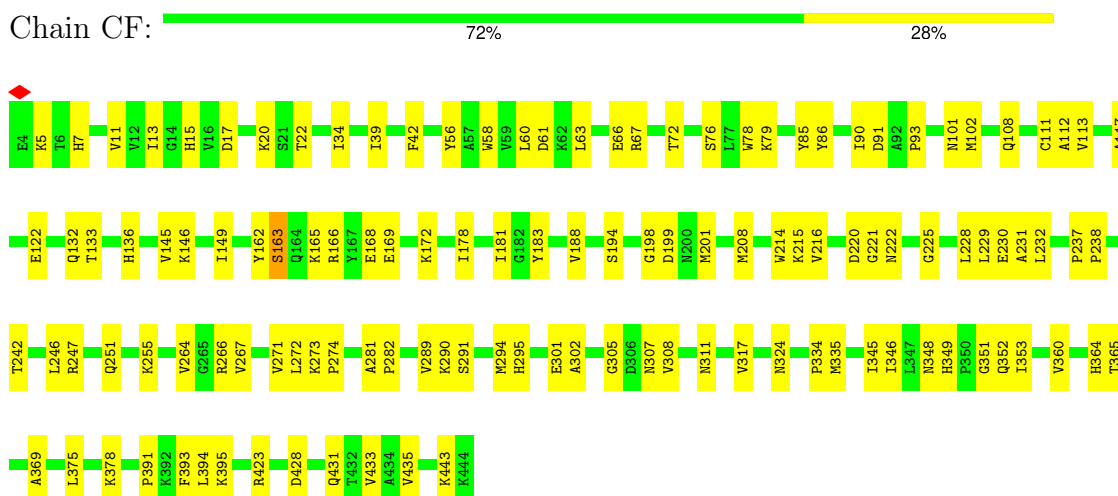
- Molecule 1: Transcription factor BTF3



- Molecule 2: P site tRNA



- Molecule 3: Elongation factor 1-alpha 1

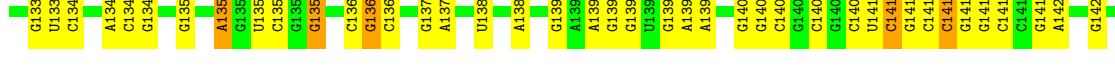
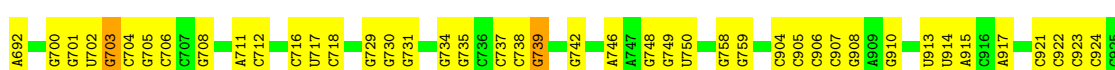
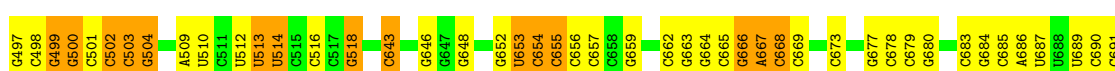
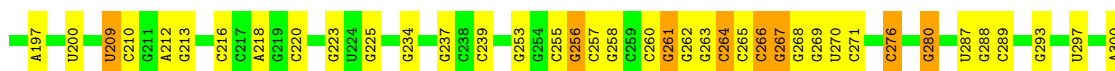
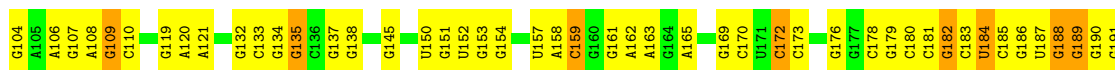
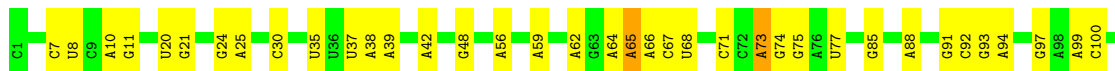


- Molecule 4: AT site tRNA



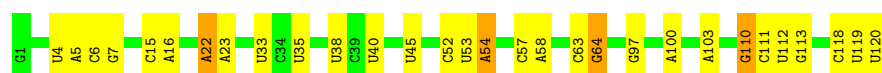


• Molecule 5: 28S rRNA

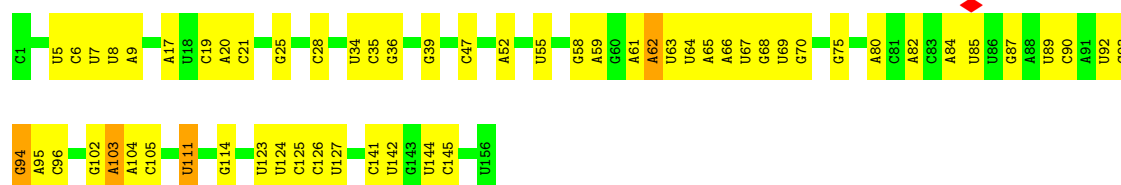


G3659	C2909	C2814	C2719	C2627	A2537	U2436	U2329	G2094	U1992	C1913	G1811	A1632
C3660	G2910	A2815	C2720	C2627	U2538	C2437	G2330	A2095	C1993	G1912	G1815	G1633
G3661	C3594	G2816	G2721	U2632	C2539	G2437	G2331	G2096	C1994	C1913	G1815	A1634
A3662	G3585			U2633	C2540	G2448	G2332	G2097	G1995	C1732	G1818	C1732
A3663	C3588	G2822	G2724	U2634	A2543	A2449	G2333	G2098	G1996	G1733	G1819	A1637
G3664	G2823	G2823	A2725	U2635	G2544	A2453	G2334	C2101	A1998	G1734	G1820	A1638
G3665	G3589	C2824	G2726	U2636	U2545		G2335	G2102	A1999	G1735	G1821	U1639
C3666	G3590	A2825		U2637	G2546		G2336	G2103	G2000		G1822	C1640
	C3591	U2826	G2732	U2638	G2547	C2458		G2104	A2002	G1739	G1823	G1641
C3670	G3592	G2827	C2733	U2639	G2547			G2105	G2003	G1740	G1824	A1642
G3673	C3593	U2828		U2640	G2547	C2464	A2347	G2106	G2004	A1742	A1825	C1645
G3674	G3594	U2829	C2739	G2640	G2550	C2465	A2348	G2107	U2004	A1743	A1825	A1646
	U3595			A2641	U2550		A2349	C2107	G2005	U1744		U1647
C3685	A3596	A2832	G2742				U2550		G2006		U1834	
G3686	C3597		A2743	G2648	U2554	U2468	C2351	C2110	U2006	G1931	G1835	G1654
A3687	G3598	A2835	A2744	G2649	G2555	C2469	G2352	G2111	G2007	A1932	G1836	C1655
U3688	A3599	U2836	A2745	U2556	G2556	G2470	A2360	G2112	U2008	G1933	A1837	
G3689	G3600	G2837	A2746	G2652	G2557	G2471	G2361	C2249	A2009	A1934	G1842	C1661
U3690	A3604	G2838		G2653	C2557		U2362	G2250	A2010	C1935		C1662
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A3692	G3606	A2844	G2750	G2655		G2475	G2364	G2252	A2012		G1847	G1667
U3693	U3607	A2845			A2565		A2368	C2256	A2017	A1942	C1848	A1668
U3694	A3608	G2846	G2756	G2658	C2568	C2478		C2257	G2018	G1948	G1855	A1669
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U3697	G3611	G2849	G2759	G2664	C2571	G2481	G2378	G2262	G2021	G1951	G1858	U1673
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U3709	G3625	G2855	A2765	G2670	A2581	G2487	U2386	G2280		G1961	U1866	A1679
G3710	U3626	U2856	U2766	G2671	C2582	G2488	U2387	U2281	G2034	A1960	A1867	G1690
A3711	G3627	G2857	U2767	G2672	C2583	G2489	A2395	G2289	G2035	G1962	G1868	
A3712		G2858	G2770	G2675	G2586	C2491	G2396	G2290	G2045		G1870	U1683
U3713	A3630	A2870		A2676	A2587	G2492	U2398	G2292	G2046	G1969	C1872	G1695
A3717	C3633	A2871	G2773	G2677	C2588	G2493	G2399	U2293	A2047		G1871	C1696
A3718	G3634			U2687	C2589	U2495	G2400	G2296	U2048	G1970	G1872	U1697
A3719	A3635	G2876	G2777	U2688	G2590	G2496	A2401	G2297	G2049	C1971	C1875	A1683
G3720	C3636	G2877	G2778	G2688	A2591	G2497	G2402	U2298	G2055	G1972	U1876	G1688
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A3723	U3639	U2891	U2787	A2695	C2603		U2408	G2301	U2061	G1975	G1879	C1698
A3726	U3640	A2894	U2789	A2696	C2607	C2504	U2409	G2302	G2062	C1977	C1879	A1786
A3727	G3641		U2790	C2702	G2610	G2505	C2410	G2303	A2069	C1978	U1882	A1787
A3732	U3644	G2898		G2706	G2611	G2506	A2411	G2306		U1979	G1890	C1703
A3733	A3645	C2899	U2803	U2707	G2612	A2513	A2412	G2306	G2076	U1980	A1891	G1705
A3734	G3646	U2900	C2804	G2708	G2613	G2514	U2413	A2313		G1981	A1892	
A3736	A3647	G2901	C2805	U2709	C2613	G2515	U2414	G2318	G2079	G1982	G1895	C1717
A3737	G3648	G2902	A2806	G2710	G2618	A2517	U2415	G2319	U2080	A1983	A1896	C1718
	U3654	G2903		G2711	G2618	G2518	A2417	G2321	C2083	A1984	A1897	A1719
G3655	G3655	U2904	G2809	G2711	A2621	G2519	G2421	G2324	C2084	G1985	G1898	G1805
A3748	U3656	C2905	U2810	G2716	G2622	U2520	G2424	G2325		U1986	G1899	U1725
G3753	U3657	G2907	A2812	G2717	A2623	G2521	G2424	G2326	G2092	C1987	G1910	U1726
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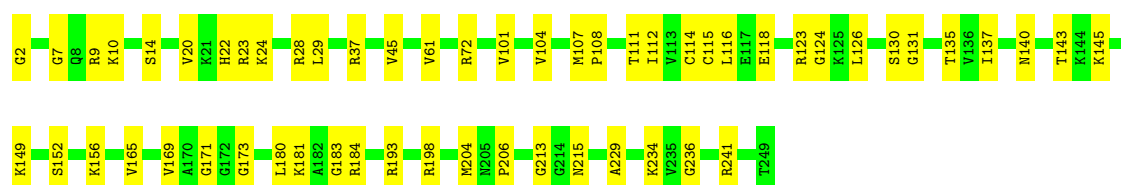
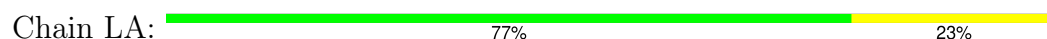




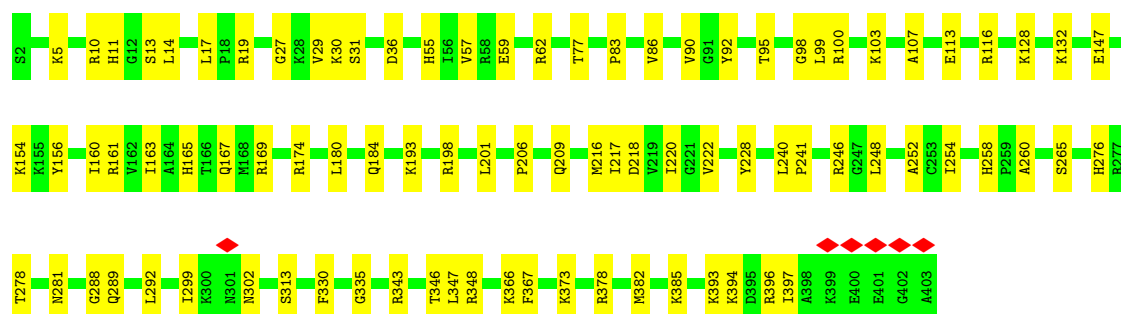
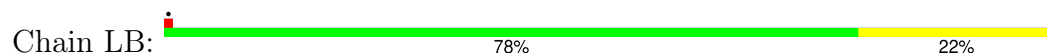
- Molecule 7: 5.8S rRNA



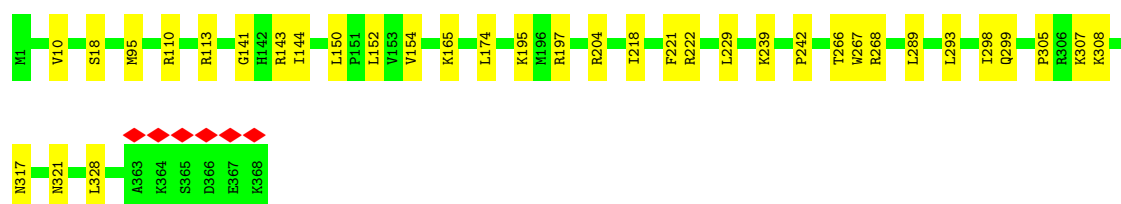
- Molecule 8: 60S ribosomal protein L8



- Molecule 9: Large ribosomal subunit protein uL3

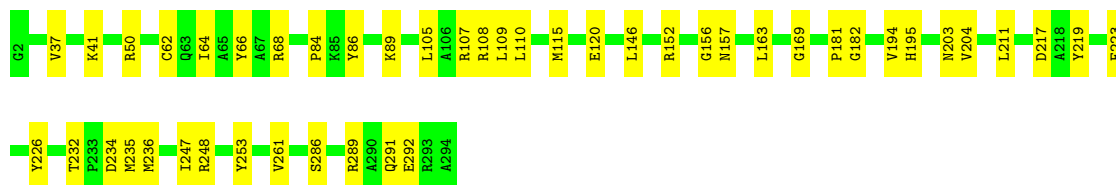


- Molecule 10: Large ribosomal subunit protein uL4



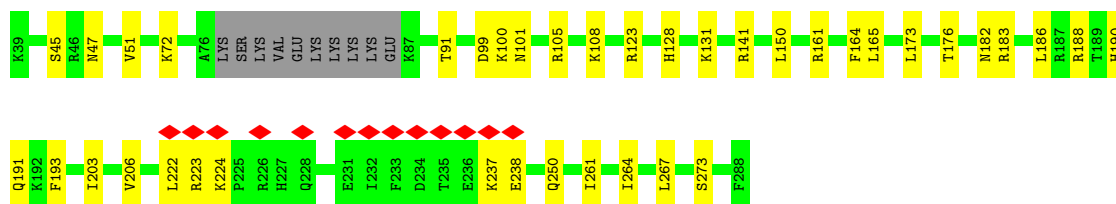
- Molecule 11: Large ribosomal subunit protein uL18

Chain LD:  84% 16%



- Molecule 12: Large ribosomal subunit protein eL6

Chain LE:  5% 80% 16%



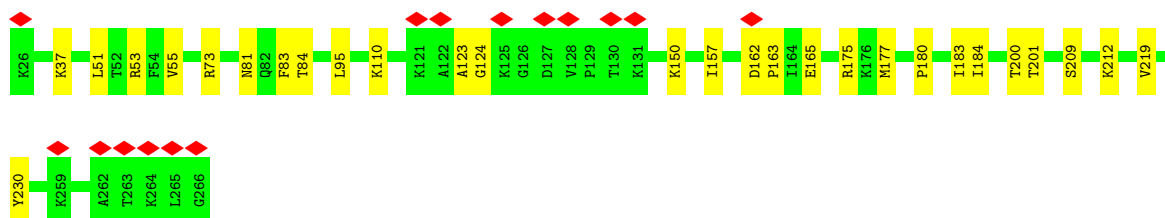
- Molecule 13: 60S ribosomal protein L7

Chain LF:  84% 16%



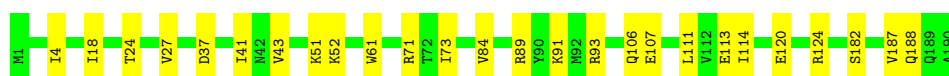
- Molecule 14: 60S ribosomal protein L7a

Chain LG:  6% 88% 12%



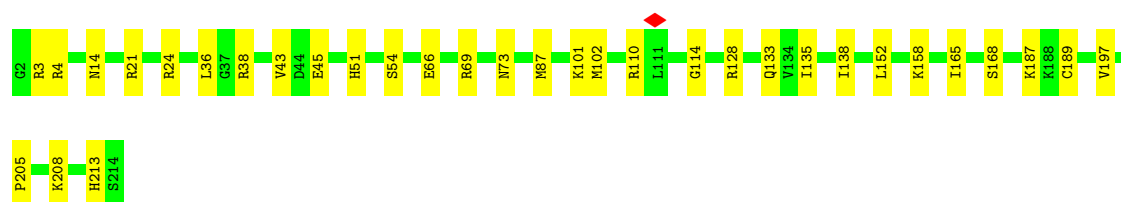
- Molecule 15: 60S ribosomal protein L9

Chain LH:  86% 14%



- Molecule 16: Ribosomal protein uL16-like

Chain LI:  85% 15%



- Molecule 17: 60S ribosomal protein L11

Chain LJ: 80% 17%



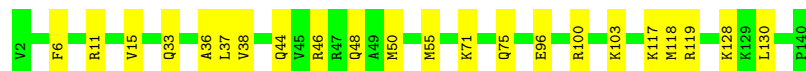
- Molecule 18: Large ribosomal subunit protein eL13

Chain LL: 90% 10%



- Molecule 19: 60S ribosomal protein L14

Chain LM: 84% 16%



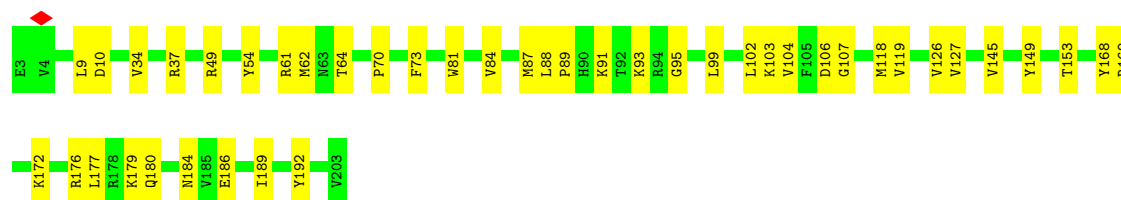
- Molecule 20: 60S ribosomal protein L15

Chain LN: 89% 11%



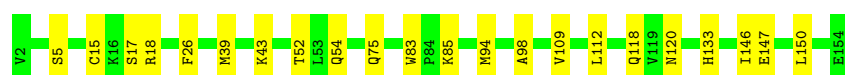
- Molecule 21: 60S ribosomal protein L13a

Chain LO: 79% 21%



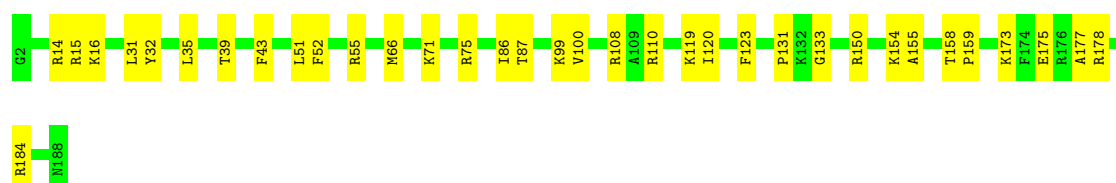
- Molecule 22: 60S ribosomal protein L17

Chain LP:  86% 14%



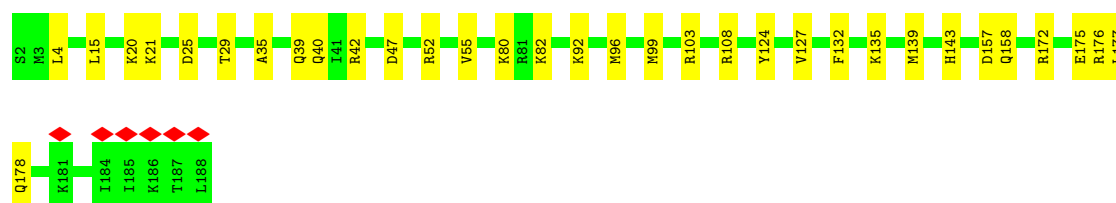
- Molecule 23: 60S ribosomal protein L18

Chain LQ:  81% 19%



- Molecule 24: 60S ribosomal protein L19

Chain LR:  82% 18%



- Molecule 25: 60S ribosomal protein L18a

Chain LS:  83% 17%



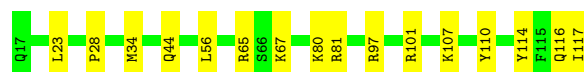
- Molecule 26: 60S ribosomal protein L21

Chain LT:  82% 18%



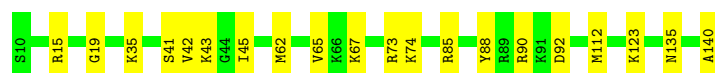
- Molecule 27: Heparin-binding protein HBp15

Chain LU:  84% 16%



- Molecule 28: 60S ribosomal protein L23

Chain LV:  85% 15%



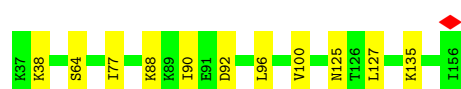
- Molecule 29: Ribosomal protein L24

Chain LW:  77% 17% 6%



- Molecule 30: 60S ribosomal protein L23a

Chain LX:  91% 9%



- Molecule 31: 60S ribosomal protein L26

Chain LY:  82% 18%



- Molecule 32: 60S ribosomal protein L27

Chain LZ:  79% 21%



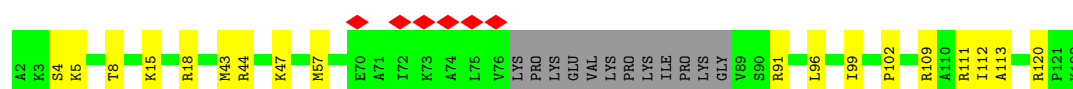
- Molecule 33: 60S ribosomal protein L27a

Chain La:  89% 11%



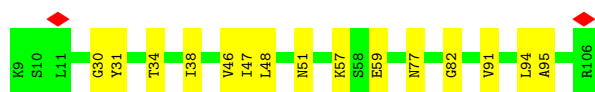
- Molecule 34: Large ribosomal subunit protein eL29

Chain Lb:  5% 75% 15% 10%



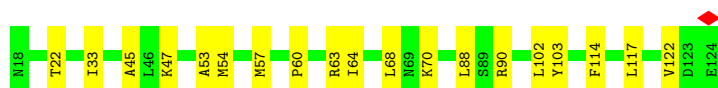
- Molecule 35: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 36: 60S ribosomal protein L31

Chain Ld:  82% 18%



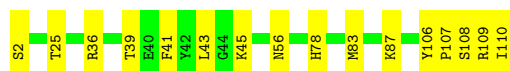
- Molecule 37: 60S ribosomal protein L32

Chain Le:  84% 16%



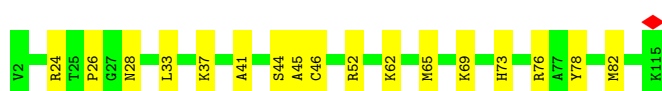
- Molecule 38: 60S ribosomal protein L35a

Chain Lf:  85% 15%



- Molecule 39: 60S ribosomal protein L34

Chain Lg:  85% 15%



- Molecule 40: 60S ribosomal protein L35

Chain Lh:  83% 17%



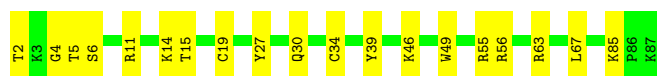
- Molecule 41: 60S ribosomal protein L36

Chain Li:  90% 10%



- Molecule 42: 60S ribosomal protein L37

Chain Lj:  78% 22%



- Molecule 43: 60S ribosomal protein L38

Chain Lk:  75% 25%



- Molecule 44: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 45: Large ribosomal subunit protein eL40

Chain Lm:  88% 12%



- Molecule 46: 60S ribosomal protein L41

Chain Ln:  79% 21%



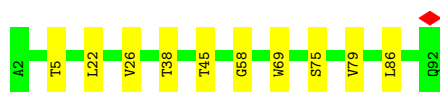
- Molecule 47: 60S ribosomal protein L36a

Chain Lo:  5% 87% 13%



- Molecule 48: 60S ribosomal protein L37a

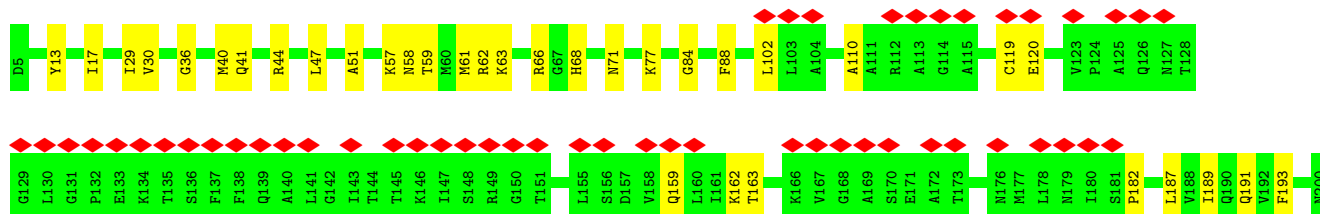
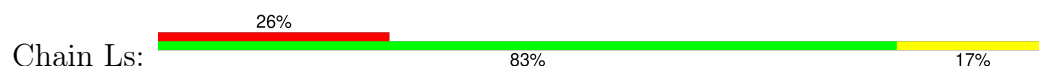
Chain Lp:  89% 11%



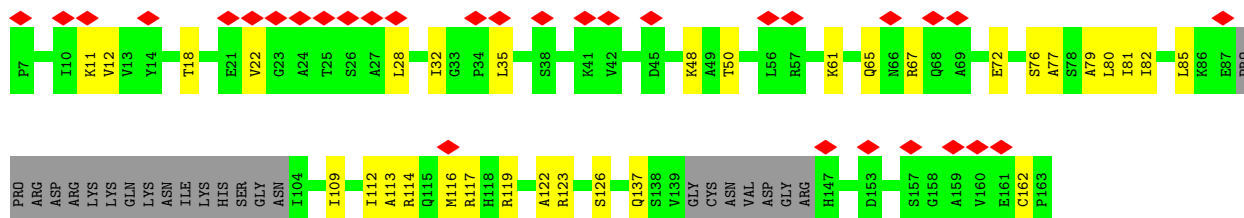
- Molecule 49: 60S ribosomal protein L28



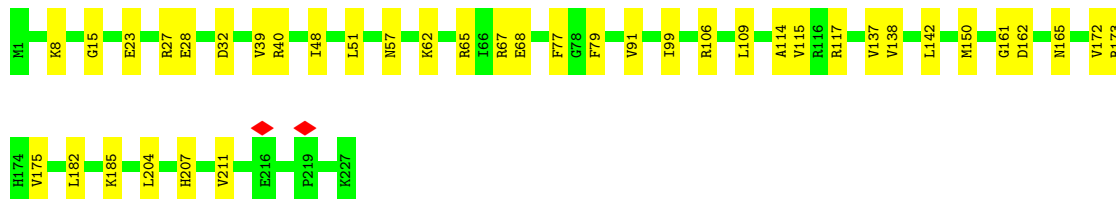
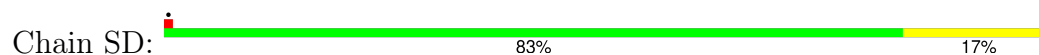
- Molecule 50: 60S acidic ribosomal protein P0



- Molecule 51: Large ribosomal subunit protein uL11

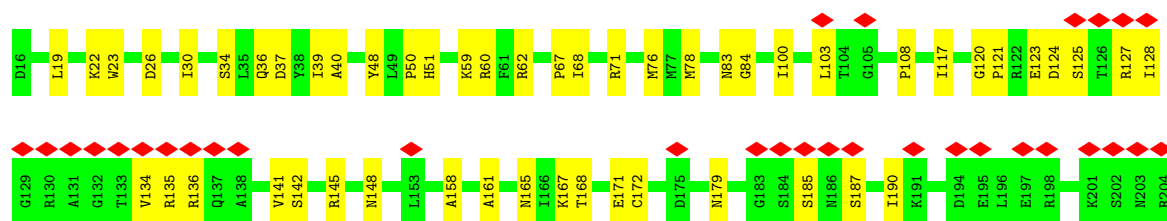


- Molecule 52: Small ribosomal subunit protein uS3



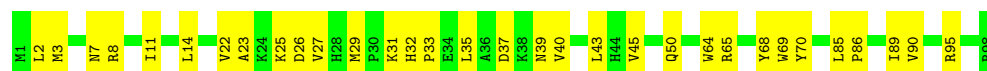
- Molecule 53: 40S ribosomal protein S5





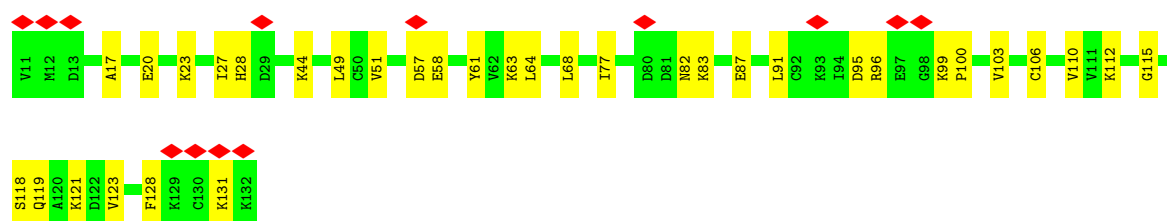
- Molecule 54: 40S ribosomal protein S10

Chain SK: 67% 33%



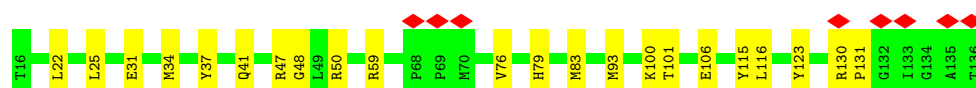
- Molecule 55: Small ribosomal subunit protein eS12

Chain SM: 11% 72% 28%



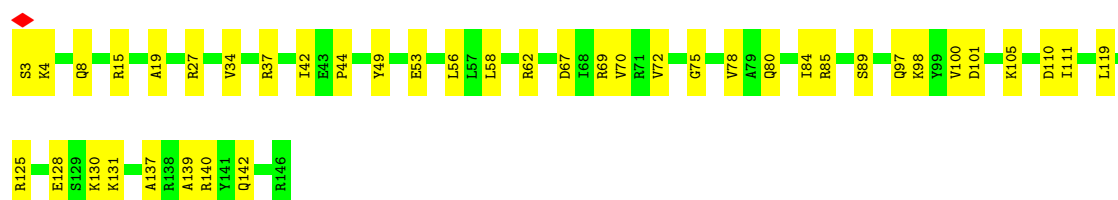
- Molecule 56: Small ribosomal subunit protein uS19

Chain SP: 7% 82% 18%



- Molecule 57: Small ribosomal subunit protein uS9

Chain SQ: 72% 28%

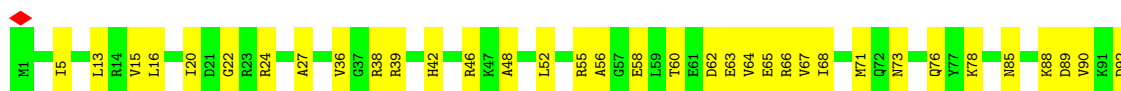


- Molecule 58: Small ribosomal subunit protein eS17

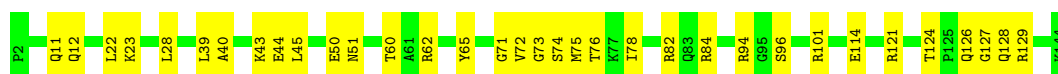
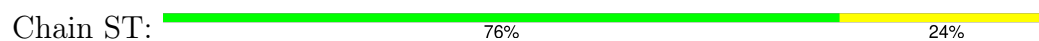
Chain SR: 87% 12%



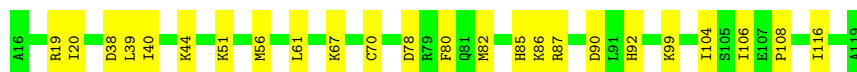
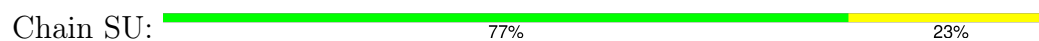
- Molecule 59: 40S ribosomal protein S18



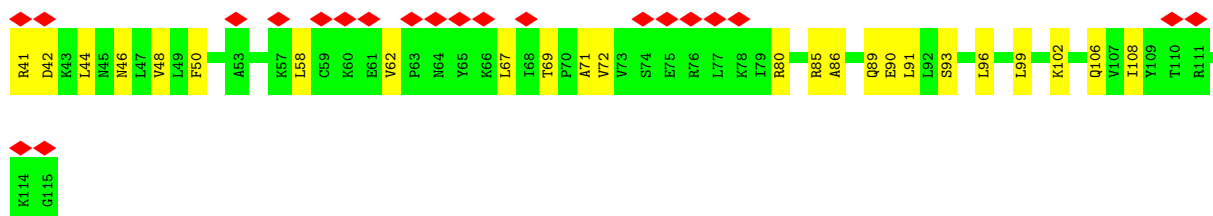
- Molecule 60: 40S ribosomal protein S19



- Molecule 61: 40S ribosomal protein S20



- Molecule 62: Small ribosomal subunit protein eS25



- Molecule 63: 40S ribosomal protein S28



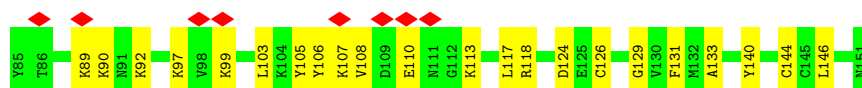
- Molecule 64: 40S ribosomal protein S29

Chain Sd:  82% 18%



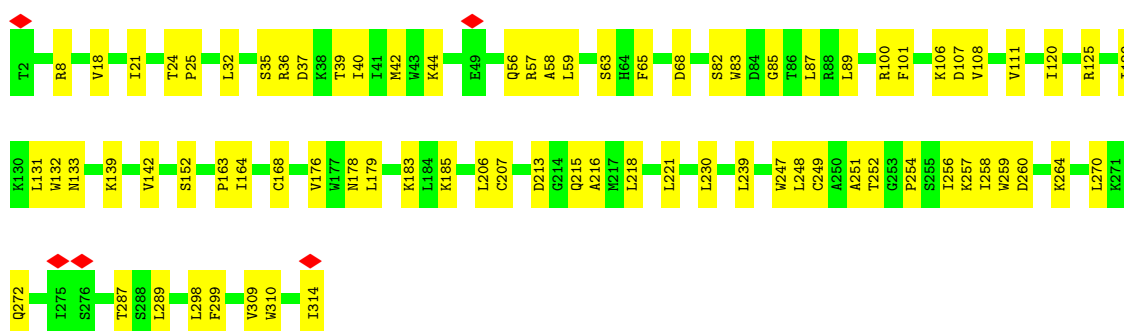
- Molecule 65: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  12% 67% 33%



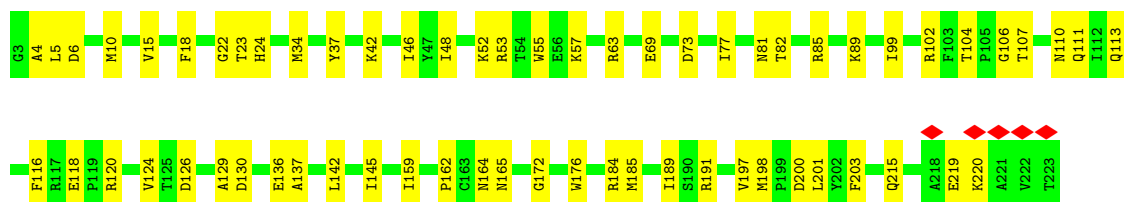
- Molecule 66: Receptor of activated protein C kinase 1

Chain Sg:  75% 25%



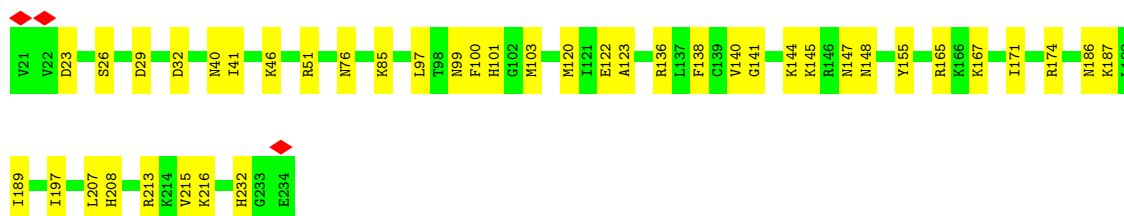
- Molecule 67: 40S ribosomal protein SA

Chain SA:  71% 29%



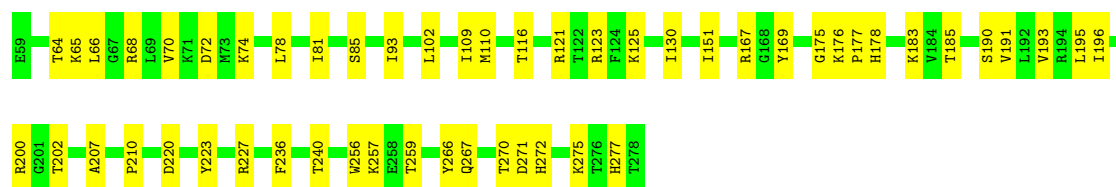
- Molecule 68: 40S ribosomal protein S3a

Chain SB:  81% 19%



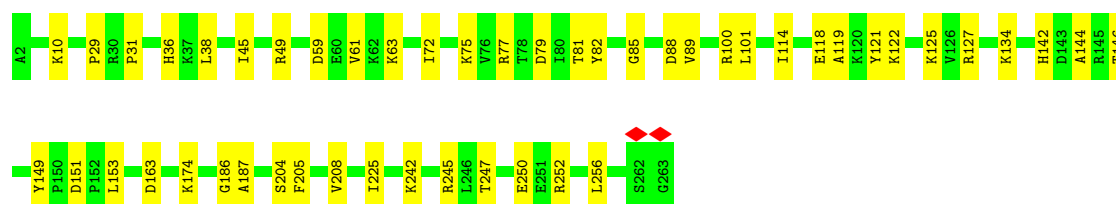
- Molecule 69: 40S ribosomal protein S2

Chain SC:  76% 24%



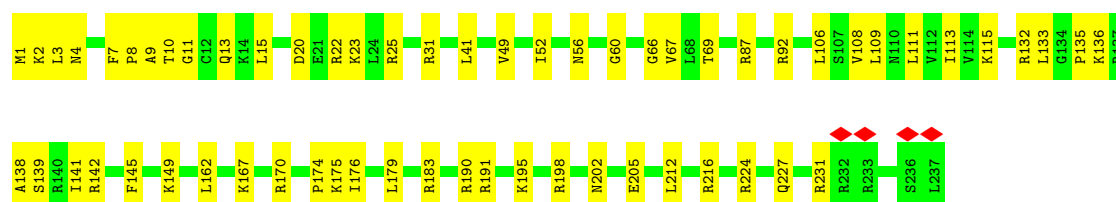
- Molecule 70: Small ribosomal subunit protein eS4, X isoform

Chain SE:  81% 19%



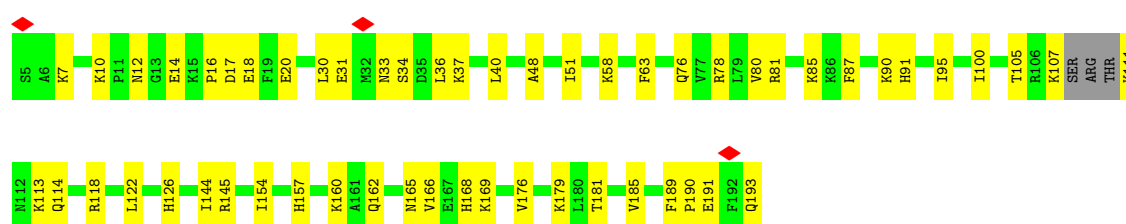
- Molecule 71: 40S ribosomal protein S6

Chain SG:  74% 26%



- Molecule 72: Small ribosomal subunit protein eS7

Chain SH:  69% 29%



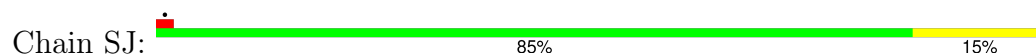
- Molecule 73: 40S ribosomal protein S8

Chain SI:  79% 21%

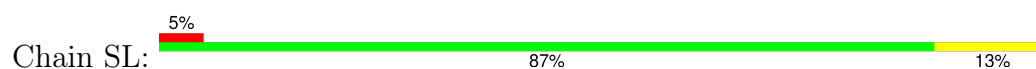




- Molecule 74: 40S ribosomal protein S9



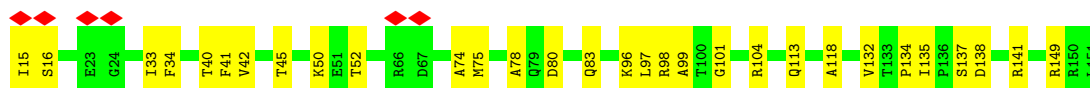
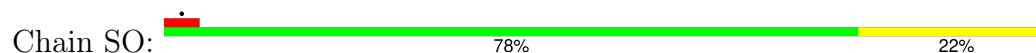
- Molecule 75: 40S ribosomal protein S11



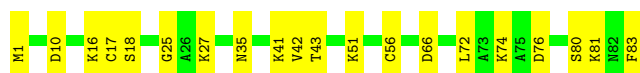
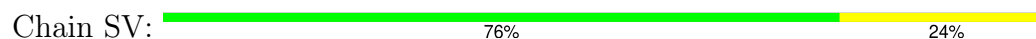
- Molecule 76: 40S ribosomal protein S13



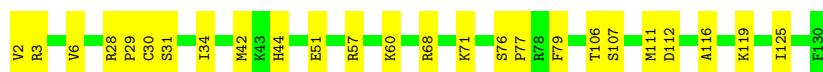
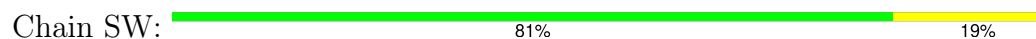
- Molecule 77: 40S ribosomal protein S14



- Molecule 78: Small ribosomal subunit protein eS21



- Molecule 79: 40S ribosomal protein S15a



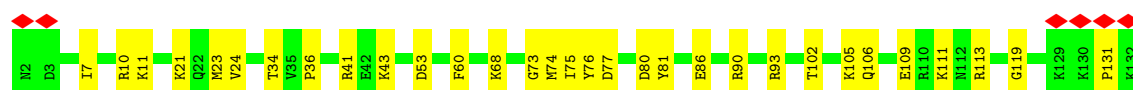
- Molecule 80: 40S ribosomal protein S23

Chain SX:  82% 18%



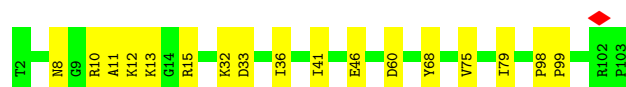
- Molecule 81: 40S ribosomal protein S24

Chain SY:  5% 76% 24%



- Molecule 82: 40S ribosomal protein S26

Chain Sa:  83% 17%



- Molecule 83: Small ribosomal subunit protein eS27

Chain Sb:  82% 18%



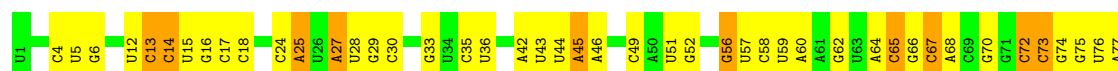
- Molecule 84: Small ribosomal subunit protein eS30

Chain Se:  12% 81% 19%



- Molecule 85: 18S rRNA

Chain S2:  49% 42% 9%





U1631	G1632	A1633	A1634	A1637	G1638	G1639	U1643	C1644	G1648	U1649	A1650	A1651	G1652	U1653	G1654	C1655	G1656	G1657	G1658	U1659	C1660	A1661	U1662	A1663	G1664	G1665	C1666	U1667	U1668					U1677	A1678	A1679	G1680	U1681	C1682	C1683	C1684	U1685	G1686	C1687	C1688	U1692	G1693	U1694	A1695	C1698	A1699		
G1705	G1706	U1707	A1715	C1716	C1717	G1718	A1719	U1720	U1721	G1722	U1729	U1730	A1731	G1732	G1736	G1737	C1738	G1744	A1745	G1748	G1749	C1750	G1751	G1752	C1753	G1754	C1755	C1756	G1757	G1758	G1759	G1760	U1761	C1762	G1763	G1764	C1767	A1768	C1769	G1770	G1771	C1772	C1773	C1774	U1775	G1776	G1777	C1778	G1779	G1780	A1781	G1782	C1783
G1784	C1785	U1786	U1797	C1798	A1801	C1802	U1803	U1804	G1805	U1808	A1809	U1810	G1814	U1821	A1825	G1826	G1829	U1830	A1831	A1832	C1833	A1834	A1835	U1838	N1842	G1843	U1844	A1845	G1846	G1849	A1850	A1851	U1854	G1855	C1856	G1857	G1858	A1859	A1860	G1861	G1862	A1863	U1864	C1865	A1869								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119172	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 4AC, 6MZ, OMG, OMU, G7M, UR3, OMC, SPM, 1MA, MA6, MG, PSU, ZN, B8N, UY1, SEP, A2M, SPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CI	0.16	0/247	0.30	0/323
2	Pt	0.13	0/1761	0.26	0/2741
3	CF	0.14	0/3442	0.40	0/4656
4	AT	0.12	0/1805	0.25	0/2809
5	L5	0.21	0/85098	0.30	1/132762 (0.0%)
6	L7	0.19	0/2861	0.25	0/4459
7	L8	0.20	0/3631	0.28	0/5657
8	LA	0.21	0/1936	0.42	0/2596
9	LB	0.20	0/3306	0.37	0/4424
10	LC	0.19	0/2981	0.36	0/4002
11	LD	0.16	0/2428	0.33	0/3252
12	LE	0.17	0/1973	0.41	0/2645
13	LF	0.18	0/1905	0.31	0/2539
14	LG	0.18	0/1960	0.39	0/2637
15	LH	0.18	0/1537	0.35	0/2066
16	LI	0.17	0/1751	0.33	0/2340
17	LJ	0.16	0/1385	0.38	0/1852
18	LL	0.17	0/1732	0.33	0/2315
19	LM	0.18	0/1161	0.37	0/1554
20	LN	0.19	0/1746	0.34	0/2338
21	LO	0.20	0/1682	0.35	0/2250
22	LP	0.20	0/1268	0.40	0/1701
23	LQ	0.20	0/1537	0.37	0/2052
24	LR	0.17	0/1582	0.35	0/2091
25	LS	0.19	0/1493	0.36	0/2003
26	LT	0.18	0/1326	0.33	0/1770
27	LU	0.18	0/839	0.45	0/1126
28	LV	0.18	0/993	0.35	0/1332
29	LW	0.17	0/959	0.38	0/1270
30	LX	0.16	0/1002	0.32	0/1345
31	LY	0.19	0/1132	0.38	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LZ	0.17	0/1130	0.35	0/1507
33	La	0.18	0/1191	0.31	0/1591
34	Lb	0.16	0/889	0.41	0/1175
35	Lc	0.18	0/774	0.38	0/1038
36	Ld	0.18	0/903	0.34	0/1216
37	Le	0.21	0/1071	0.38	0/1429
38	Lf	0.20	0/895	0.37	0/1198
39	Lg	0.18	0/916	0.34	0/1220
40	Lh	0.16	0/1023	0.32	0/1351
41	Li	0.16	0/843	0.35	0/1115
42	Lj	0.19	0/720	0.36	0/952
43	Lk	0.19	0/575	0.47	0/761
44	Ll	0.17	0/454	0.29	0/599
45	Lm	0.17	0/435	0.36	0/575
46	Ln	0.16	0/231	0.31	0/294
47	Lo	0.17	0/876	0.35	0/1156
48	Lp	0.17	0/718	0.32	0/953
49	Lr	0.17	0/1017	0.33	0/1364
50	Ls	0.12	0/1519	0.34	0/2052
51	Lt	0.16	0/1009	0.50	0/1363
52	SD	0.13	0/1793	0.30	0/2414
53	SF	0.15	0/1516	0.36	0/2037
54	SK	0.16	0/851	0.43	0/1147
55	SM	0.14	0/950	0.40	0/1275
56	SP	0.17	0/1003	0.40	0/1342
57	SQ	0.15	0/1160	0.39	0/1553
58	SR	0.16	0/1105	0.45	0/1484
59	SS	0.14	0/1216	0.37	0/1628
60	ST	0.15	0/1131	0.40	0/1515
61	SU	0.17	0/831	0.47	0/1115
62	SZ	0.17	0/604	0.48	0/810
63	Sc	0.16	0/508	0.40	0/680
64	Sd	0.14	0/470	0.37	0/623
65	Sf	0.16	0/560	0.48	0/745
66	Sg	0.13	0/2493	0.38	0/3394
67	SA	0.15	0/1778	0.35	0/2416
68	SB	0.14	0/1765	0.37	0/2362
69	SC	0.15	0/1744	0.34	0/2357
70	SE	0.14	0/2118	0.37	0/2849
71	SG	0.15	0/1946	0.37	0/2590
72	SH	0.16	0/1519	0.41	0/2033
73	SI	0.16	0/1715	0.37	0/2287
74	SJ	0.13	0/1550	0.32	0/2069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SL	0.15	0/1268	0.34	0/1696
76	SN	0.13	0/1232	0.29	0/1656
77	SO	0.17	0/1037	0.39	0/1391
78	SV	0.16	0/643	0.39	0/860
79	SW	0.18	0/1051	0.38	0/1406
80	SX	0.15	0/1116	0.35	0/1490
81	SY	0.15	0/1083	0.40	0/1438
82	Sa	0.15	0/836	0.33	0/1121
83	Sb	0.16	0/665	0.37	0/891
84	Se	0.14	0/465	0.38	0/612
85	S2	0.18	0/39756	0.28	0/61939
All	All	0.19	0/235126	0.32	1/344545 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
77	SO	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	1703	C	C2'-C3'-O3'	5.16	117.24	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
77	SO	137	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	14	0
2	Pt	1576	0	803	20	0
3	CF	3383	0	3431	80	0
4	AT	1616	0	824	30	0
5	L5	78444	0	39718	961	0
6	L7	2561	0	1295	16	0
7	L8	3315	0	1685	36	0
8	LA	1898	0	1993	44	0
9	LB	3238	0	3376	67	0
10	LC	2927	0	3104	28	0
11	LD	2382	0	2410	31	0
12	LE	1935	0	2096	29	0
13	LF	1870	0	1996	28	0
14	LG	1927	0	2074	17	0
15	LH	1518	0	1601	19	0
16	LI	1711	0	1749	22	0
17	LJ	1362	0	1399	18	0
18	LL	1701	0	1818	22	0
19	LM	1138	0	1204	16	0
20	LN	1701	0	1749	21	0
21	LO	1650	0	1794	32	0
22	LP	1242	0	1269	16	0
23	LQ	1513	0	1628	26	0
24	LR	1566	0	1729	26	0
25	LS	1453	0	1490	20	0
26	LT	1298	0	1366	23	0
27	LU	825	0	850	14	0
28	LV	979	0	1039	14	0
29	LW	945	0	1003	18	0
30	LX	985	0	1066	8	0
31	LY	1115	0	1205	16	0
32	LZ	1107	0	1182	17	0
33	La	1162	0	1213	12	0
34	Lb	876	0	948	16	0
35	Lc	764	0	804	8	0
36	Ld	888	0	930	11	0
37	Le	1053	0	1147	16	0
38	Lf	876	0	912	10	0
39	Lg	906	0	998	16	0
40	Lh	1015	0	1148	19	0
41	Li	832	0	917	7	0
42	Lj	705	0	737	19	0
43	Lk	569	0	637	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ll	444	0	483	11	0
45	Lm	429	0	465	5	0
46	Ln	230	0	276	4	0
47	Lo	862	0	929	10	0
48	Lp	708	0	756	9	0
49	Lr	1002	0	1068	4	0
50	Ls	1496	0	1540	22	0
51	Lt	998	0	1032	26	0
52	SD	1765	0	1865	27	0
53	SF	1495	0	1549	38	0
54	SK	827	0	854	23	0
55	SM	940	0	965	21	0
56	SP	985	0	1031	17	0
57	SQ	1142	0	1213	31	0
58	SR	1090	0	1149	13	0
59	SS	1198	0	1261	33	0
60	ST	1112	0	1146	24	0
61	SU	821	0	883	17	0
62	SZ	598	0	656	19	0
63	Sc	506	0	536	14	0
64	Sd	459	0	452	10	0
65	Sf	548	0	551	17	0
66	Sg	2436	0	2393	50	0
67	SA	1741	0	1746	48	0
68	SB	1738	0	1809	25	0
69	SC	1707	0	1791	39	0
70	SE	2076	0	2177	33	0
71	SG	1923	0	2089	60	0
72	SH	1497	0	1590	40	0
73	SI	1686	0	1772	34	0
74	SJ	1525	0	1640	22	0
75	SL	1247	0	1323	13	0
76	SN	1208	0	1294	14	0
77	SO	1024	0	1050	19	0
78	SV	636	0	637	16	0
79	SW	1034	0	1080	24	0
80	SX	1098	0	1167	22	0
81	SY	1065	0	1142	22	0
82	Sa	821	0	870	12	0
83	Sb	651	0	672	13	0
84	Se	459	0	503	11	0
85	S2	36953	0	18678	537	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L5	178	0	0	0	0
86	L7	3	0	0	0	0
86	L8	4	0	0	0	0
86	LA	1	0	0	0	0
86	LB	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	Lj	1	0	0	0	0
86	S2	26	0	0	0	0
86	SG	1	0	0	0	0
86	SS	1	0	0	0	0
87	L5	98	0	182	4	0
88	L5	90	0	171	3	0
88	LN	10	0	19	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
All	All	223377	0	167075	2774	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2774 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:79:ARG:NH1	5:L5:2708:U:O2'	1.64	1.29
5:L5:1996:C:H42	5:L5:2000:G:H22	1.10	0.98
5:L5:1996:C:H42	5:L5:2000:G:N2	1.66	0.93
5:L5:4946:U:HO2'	38:Lf:2:SER:N	1.67	0.92
1:CI:74:LYS:HA	27:LU:116:GLN:O	1.68	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
3	CF	438/441 (99%)	420 (96%)	18 (4%)	0	100	100
8	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
9	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
10	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
11	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
12	LE	236/250 (94%)	221 (94%)	15 (6%)	0	100	100
13	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
14	LG	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
15	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
16	LI	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
17	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
18	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
19	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
20	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
21	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
22	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
23	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
24	LR	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
25	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
26	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
27	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
28	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
29	LW	112/124 (90%)	108 (96%)	4 (4%)	0	100	100
30	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
32	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
33	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
34	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
35	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
36	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
37	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
38	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
39	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
40	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
41	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
42	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
43	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
44	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
45	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
46	Ln	22/24 (92%)	22 (100%)	0	0	100	100
47	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
48	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
49	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
50	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
51	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
52	SD	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
53	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
54	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
55	SM	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
56	SP	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
57	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
58	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	31
59	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
60	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
61	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SZ	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
63	Sc	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
64	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
65	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
66	Sg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
67	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
68	SB	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
69	SC	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
70	SE	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
71	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
72	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
73	SI	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
74	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	43
75	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
76	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
77	SO	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
78	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
79	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
80	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
81	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
82	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
83	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
84	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
All	All	12110/12343 (98%)	11574 (96%)	534 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	SR	129	LYS
74	SJ	138	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
3	CF	365/366 (100%)	365 (100%)	0	100	100
8	LA	190/190 (100%)	190 (100%)	0	100	100
9	LB	348/348 (100%)	348 (100%)	0	100	100
10	LC	306/306 (100%)	306 (100%)	0	100	100
11	LD	246/247 (100%)	246 (100%)	0	100	100
12	LE	212/222 (96%)	212 (100%)	0	100	100
13	LF	194/194 (100%)	194 (100%)	0	100	100
14	LG	203/205 (99%)	203 (100%)	0	100	100
15	LH	169/169 (100%)	169 (100%)	0	100	100
16	LI	180/180 (100%)	180 (100%)	0	100	100
17	LJ	143/148 (97%)	143 (100%)	0	100	100
18	LL	176/176 (100%)	176 (100%)	0	100	100
19	LM	118/118 (100%)	118 (100%)	0	100	100
20	LN	171/171 (100%)	171 (100%)	0	100	100
21	LO	173/173 (100%)	173 (100%)	0	100	100
22	LP	134/134 (100%)	134 (100%)	0	100	100
23	LQ	164/164 (100%)	164 (100%)	0	100	100
24	LR	166/166 (100%)	166 (100%)	0	100	100
25	LS	156/156 (100%)	156 (100%)	0	100	100
26	LT	139/139 (100%)	139 (100%)	0	100	100
27	LU	91/91 (100%)	91 (100%)	0	100	100
28	LV	101/101 (100%)	101 (100%)	0	100	100
29	LW	95/103 (92%)	95 (100%)	0	100	100
30	LX	108/108 (100%)	108 (100%)	0	100	100
31	LY	124/124 (100%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	LZ	117/117 (100%)	117 (100%)	0	100	100
33	La	120/120 (100%)	120 (100%)	0	100	100
34	Lb	88/101 (87%)	88 (100%)	0	100	100
35	Lc	83/83 (100%)	83 (100%)	0	100	100
36	Ld	98/98 (100%)	98 (100%)	0	100	100
37	Le	114/114 (100%)	114 (100%)	0	100	100
38	Lf	88/88 (100%)	88 (100%)	0	100	100
39	Lg	98/98 (100%)	98 (100%)	0	100	100
40	Lh	109/109 (100%)	109 (100%)	0	100	100
41	Li	86/86 (100%)	86 (100%)	0	100	100
42	Lj	73/73 (100%)	73 (100%)	0	100	100
43	Lk	64/64 (100%)	64 (100%)	0	100	100
44	Ll	47/47 (100%)	47 (100%)	0	100	100
45	Lm	48/48 (100%)	48 (100%)	0	100	100
46	Ln	23/23 (100%)	23 (100%)	0	100	100
47	Lo	93/93 (100%)	93 (100%)	0	100	100
48	Lp	74/74 (100%)	74 (100%)	0	100	100
49	Lr	109/109 (100%)	109 (100%)	0	100	100
50	Ls	162/164 (99%)	162 (100%)	0	100	100
51	Lt	107/130 (82%)	107 (100%)	0	100	100
52	SD	190/190 (100%)	190 (100%)	0	100	100
53	SF	159/159 (100%)	159 (100%)	0	100	100
54	SK	89/89 (100%)	89 (100%)	0	100	100
55	SM	102/104 (98%)	102 (100%)	0	100	100
56	SP	107/107 (100%)	107 (100%)	0	100	100
57	SQ	119/119 (100%)	119 (100%)	0	100	100
58	SR	122/122 (100%)	122 (100%)	0	100	100
59	SS	126/126 (100%)	126 (100%)	0	100	100
60	ST	113/113 (100%)	113 (100%)	0	100	100
61	SU	94/94 (100%)	94 (100%)	0	100	100
62	SZ	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	Sc	57/57 (100%)	57 (100%)	0	100	100
64	Sd	48/48 (100%)	48 (100%)	0	100	100
65	Sf	60/60 (100%)	60 (100%)	0	100	100
66	Sg	272/272 (100%)	272 (100%)	0	100	100
67	SA	183/183 (100%)	183 (100%)	0	100	100
68	SB	195/195 (100%)	195 (100%)	0	100	100
69	SC	186/186 (100%)	186 (100%)	0	100	100
70	SE	224/224 (100%)	224 (100%)	0	100	100
71	SG	207/207 (100%)	207 (100%)	0	100	100
72	SH	166/169 (98%)	166 (100%)	0	100	100
73	SI	178/178 (100%)	178 (100%)	0	100	100
74	SJ	161/161 (100%)	161 (100%)	0	100	100
75	SL	137/137 (100%)	137 (100%)	0	100	100
76	SN	130/130 (100%)	130 (100%)	0	100	100
77	SO	107/107 (100%)	107 (100%)	0	100	100
78	SV	67/67 (100%)	67 (100%)	0	100	100
79	SW	112/112 (100%)	112 (100%)	0	100	100
80	SX	113/113 (100%)	113 (100%)	0	100	100
81	SY	113/113 (100%)	113 (100%)	0	100	100
82	Sa	89/89 (100%)	89 (100%)	0	100	100
83	Sb	75/75 (100%)	75 (100%)	0	100	100
84	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10512/10582 (99%)	10512 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
60	ST	63	HIS
68	SB	118	GLN
62	SZ	89	GLN
66	Sg	272	GLN
69	SC	267	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	15 (20%)	0
4	AT	74/76 (97%)	27 (36%)	0
5	L5	3643/3655 (99%)	731 (20%)	16 (0%)
6	L7	119/120 (99%)	11 (9%)	0
7	L8	155/156 (99%)	21 (13%)	0
85	S2	1714/1740 (98%)	378 (22%)	4 (0%)
All	All	5777/5821 (99%)	1183 (20%)	20 (0%)

5 of 1183 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G
2	Pt	21	A
2	Pt	46	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L5	4699	U
85	S2	563	G
85	S2	1477	U
85	S2	688	U
5	L5	1703	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

179 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	OMC	L5	1340	5	19,22,23	0.59	0	25,31,34	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	A2M	S2	1031	85	22,25,26	1.15	1 (4%)	30,36,39	1.58	7 (23%)
85	PSU	S2	1177	85	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
5	PSU	L5	4579	5	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)
5	PSU	L5	3920	5,86	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
5	PSU	L5	1536	5	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4521	5,86	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
5	OMG	L5	3627	5	23,26,27	0.49	0	32,38,41	0.60	0
5	PSU	L5	4973	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
85	OMU	S2	1288	85	19,22,23	3.39	7 (36%)	25,31,34	1.75	5 (20%)
5	PSU	L5	1744	5,86	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
5	OMG	L5	4499	5	23,26,27	0.49	0	32,38,41	0.47	0
85	PSU	S2	93	85	18,21,22	1.09	1 (5%)	21,30,33	1.78	4 (19%)
5	OMU	L5	4306	5	19,22,23	3.31	7 (36%)	25,31,34	1.82	4 (16%)
85	4AC	S2	1337	85	21,24,25	0.38	0	28,34,37	0.71	1 (3%)
5	OMC	L5	2824	5	19,22,23	0.55	0	25,31,34	0.63	0
85	OMG	S2	683	85	23,26,27	0.48	0	32,38,41	0.50	0
85	PSU	S2	651	85	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
85	OMG	S2	436	85	23,26,27	0.47	0	32,38,41	0.53	0
5	A2M	L5	398	5	22,25,26	1.15	1 (4%)	30,36,39	1.60	7 (23%)
5	A2M	L5	4523	5,86	22,25,26	1.21	2 (9%)	30,36,39	1.61	8 (26%)
5	PSU	L5	3695	5	18,21,22	1.07	1 (5%)	21,30,33	1.90	5 (23%)
5	PSU	L5	4500	5	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
5	PSU	L5	4972	5	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4471	5	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
5	OMG	L5	4228	5	23,26,27	0.49	0	32,38,41	0.62	0
5	A2M	L5	3867	5	22,25,26	1.14	1 (4%)	30,36,39	1.46	8 (26%)
5	UR3	L5	4530	5	19,22,23	2.72	7 (36%)	26,32,35	1.60	3 (11%)
85	OMU	S2	1326	85	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
5	PSU	L5	2632	5	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
85	OMC	S2	1391	85	19,22,23	0.52	0	25,31,34	0.68	0
85	OMU	S2	116	85	19,22,23	3.36	7 (36%)	25,31,34	1.77	4 (16%)
5	PSU	L5	2839	5	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
85	6MZ	S2	1832	85,86	26,26,26	2.82	5 (19%)	36,39,39	2.06	9 (25%)
5	OMC	L5	3701	5	19,22,23	0.68	0	25,31,34	1.68	4 (16%)
5	OMC	L5	3887	5	19,22,23	0.57	0	25,31,34	0.77	0
5	PSU	L5	1782	5	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	UY1	L5	3818	5	19,22,23	4.90	9 (47%)	21,31,34	1.92	5 (23%)
5	PSU	L5	4552	5	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
85	PSU	S2	406	85	18,21,22	1.11	1 (5%)	21,30,33	1.98	5 (23%)
5	PSU	L5	1860	5	18,21,22	1.03	1 (5%)	21,30,33	1.85	4 (19%)
85	A2M	S2	576	85	22,25,26	1.19	1 (4%)	30,36,39	1.53	7 (23%)
5	OMC	L5	2861	5	19,22,23	0.56	0	25,31,34	0.80	1 (4%)
5	PSU	L5	4689	5	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
5	PSU	L5	1677	5	18,21,22	1.06	1 (5%)	21,30,33	1.87	3 (14%)
5	A2M	L5	1323	5	22,25,26	1.16	2 (9%)	30,36,39	1.58	9 (30%)
5	PSU	L5	1582	5	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
5	A2M	L5	3785	5,86	22,25,26	1.08	1 (4%)	30,36,39	1.61	9 (30%)
5	OMC	L5	3869	5	19,22,23	0.60	0	25,31,34	0.70	0
7	OMG	L8	75	7	23,26,27	0.48	0	32,38,41	0.51	0
5	PSU	L5	3884	5	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
5	PSU	L5	1862	5	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
5	OMC	L5	2351	5,86	19,22,23	0.62	0	25,31,34	1.18	2 (8%)
5	6MZ	L5	4220	5	22,25,26	3.98	11 (50%)	29,36,39	2.37	11 (37%)
5	OMG	L5	2424	5	23,26,27	0.51	0	32,38,41	0.45	0
5	OMC	L5	2804	5	19,22,23	0.61	0	25,31,34	0.88	1 (4%)
85	PSU	S2	109	85	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
5	A2M	L5	2815	5	22,25,26	1.16	1 (4%)	30,36,39	1.50	8 (26%)
85	PSU	S2	105	85	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
85	OMU	S2	799	85	19,22,23	3.39	7 (36%)	25,31,34	1.81	5 (20%)
85	PSU	S2	801	85	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
85	OMG	S2	867	85	23,26,27	0.50	0	32,38,41	0.46	0
85	A2M	S2	1383	85	22,25,26	1.17	1 (4%)	30,36,39	1.61	5 (16%)
5	OMG	L5	4494	5	23,26,27	0.51	0	32,38,41	0.54	0
5	A2M	L5	400	5	22,25,26	1.18	1 (4%)	30,36,39	1.59	9 (30%)
85	A2M	S2	159	85	22,25,26	1.20	1 (4%)	30,36,39	1.52	9 (30%)
85	OMG	S2	509	85	23,26,27	0.48	0	32,38,41	0.51	0
85	PSU	S2	686	85	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
5	A2M	L5	4590	5	22,25,26	1.16	1 (4%)	30,36,39	1.53	6 (20%)
85	PSU	S2	1232	85	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
85	PSU	S2	866	85	18,21,22	1.09	1 (5%)	21,30,33	1.81	5 (23%)
5	PSU	L5	5001	5	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
5	PSU	L5	3853	5,86	18,21,22	1.04	1 (5%)	21,30,33	1.81	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	A2M	S2	166	85	22,25,26	1.28	2 (9%)	30,36,39	1.53	7 (23%)
5	PSU	L5	4353	5	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
85	OMU	S2	121	85	19,22,23	3.34	7 (36%)	25,31,34	1.85	5 (20%)
85	OMU	S2	1442	85	19,22,23	3.40	7 (36%)	25,31,34	1.82	5 (20%)
85	PSU	S2	814	85	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
5	A2M	L5	4571	5	22,25,26	1.20	1 (4%)	30,36,39	1.54	7 (23%)
85	OMG	S2	644	85	23,26,27	0.46	0	32,38,41	0.48	0
85	PSU	S2	681	85	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
5	OMG	L5	4392	5	23,26,27	0.51	0	32,38,41	0.46	0
85	OMU	S2	627	85	19,22,23	3.41	7 (36%)	25,31,34	1.82	4 (16%)
5	OMC	L5	2422	5,86	19,22,23	0.58	0	25,31,34	0.69	0
5	OMC	L5	4536	5	19,22,23	0.59	0	25,31,34	0.69	0
5	PSU	L5	4673	5,86	18,21,22	1.05	1 (5%)	21,30,33	1.82	4 (19%)
85	OMC	S2	1703	85	19,22,23	0.55	0	25,31,34	0.60	0
85	OMC	S2	517	85	19,22,23	0.53	0	25,31,34	0.64	0
5	PSU	L5	1781	5	18,21,22	1.05	1 (5%)	21,30,33	1.78	4 (19%)
5	PSU	L5	4457	5	18,21,22	1.04	1 (5%)	21,30,33	1.96	5 (23%)
85	PSU	S2	1056	85	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
5	A2M	L5	3718	5	22,25,26	1.11	1 (4%)	30,36,39	1.51	5 (16%)
5	OMG	L5	2876	5	23,26,27	0.51	0	32,38,41	0.55	0
5	A2M	L5	3830	5	22,25,26	1.13	1 (4%)	30,36,39	1.58	7 (23%)
85	PSU	S2	1004	85	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
85	PSU	S2	1367	85	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
5	A2M	L5	2401	5	22,25,26	1.16	1 (4%)	30,36,39	1.59	6 (20%)
5	PSU	L5	4442	5	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
85	OMU	S2	354	85	19,22,23	3.33	7 (36%)	25,31,34	1.88	5 (20%)
85	A2M	S2	27	85	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
85	PSU	S2	863	85	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
5	OMU	L5	2837	5	19,22,23	3.36	7 (36%)	25,31,34	1.86	4 (16%)
5	OMG	L5	1316	5	23,26,27	0.52	0	32,38,41	0.57	0
5	OMU	L5	4227	5	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
85	PSU	S2	1174	85	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
85	PSU	S2	1244	85	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4431	5	18,21,22	1.04	1 (5%)	21,30,33	1.87	4 (19%)
85	PSU	S2	1045	85	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
5	OMG	L5	3744	5	23,26,27	0.49	0	32,38,41	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	PSU	S2	1046	85	18,21,22	1.12	1 (5%)	21,30,33	1.83	4 (19%)
85	OMC	S2	174	85	19,22,23	0.53	0	25,31,34	0.65	0
85	OMU	S2	172	85	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
5	A2M	L5	2787	5	22,25,26	1.15	1 (4%)	30,36,39	1.50	8 (26%)
85	OMG	S2	1490	85	23,26,27	0.50	0	32,38,41	0.46	0
5	PSU	L5	3637	5	18,21,22	1.06	1 (5%)	21,30,33	2.02	5 (23%)
5	OMG	L5	4618	5	23,26,27	0.50	0	32,38,41	0.53	0
85	PSU	S2	649	85	18,21,22	1.08	1 (5%)	21,30,33	1.93	3 (14%)
5	PSU	L5	5010	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
85	OMG	S2	601	85	23,26,27	0.47	0	32,38,41	0.44	0
7	PSU	L8	69	7	18,21,22	1.08	1 (5%)	21,30,33	1.82	5 (23%)
5	OMG	L5	4623	5	23,26,27	0.52	0	32,38,41	0.58	0
85	B8N	S2	1248	85	25,29,30	3.28	6 (24%)	28,42,45	2.03	7 (25%)
5	1MA	L5	1322	5,86	21,25,26	0.55	0	30,37,40	0.78	1 (3%)
5	PSU	L5	4299	5	18,21,22	1.01	1 (5%)	21,30,33	1.81	4 (19%)
5	OMU	L5	4498	5	19,22,23	3.34	7 (36%)	25,31,34	1.86	5 (20%)
5	PSU	L5	4532	5	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
7	PSU	L8	55	7	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
5	PSU	L5	1792	5	18,21,22	1.02	1 (5%)	21,30,33	1.89	3 (14%)
5	5MC	L5	3782	5,86	19,22,23	0.60	0	26,32,35	0.71	0
5	OMG	L5	3899	5	23,26,27	0.54	0	32,38,41	0.51	0
5	PSU	L5	3822	5	18,21,22	1.06	1 (5%)	21,30,33	1.82	5 (23%)
5	A2M	L5	1871	5,86	22,25,26	1.17	1 (4%)	30,36,39	1.63	6 (20%)
5	A2M	L5	1326	5	22,25,26	1.14	1 (4%)	30,36,39	1.47	9 (30%)
5	PSU	L5	4361	5	18,21,22	1.01	1 (5%)	21,30,33	1.80	3 (14%)
85	OMG	S2	1328	85	23,26,27	0.46	0	32,38,41	0.45	0
5	A2M	L5	2363	5,86	22,25,26	1.15	2 (9%)	30,36,39	1.57	8 (26%)
5	PSU	L5	1683	5	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
85	G7M	S2	1639	85,2	23,26,27	2.66	8 (34%)	34,39,42	2.63	11 (32%)
5	OMG	L5	1522	5	23,26,27	0.52	0	32,38,41	0.57	0
3	SEP	CF	163	3	8,9,10	1.61	1 (12%)	7,12,14	1.30	1 (14%)
5	OMU	L5	4620	5	19,22,23	3.24	7 (36%)	25,31,34	1.75	5 (20%)
5	PSU	L5	4296	5	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
5	OMG	L5	4637	5	23,26,27	0.50	0	32,38,41	0.48	0
85	OMU	S2	428	85	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
85	A2M	S2	484	85	22,25,26	1.17	1 (4%)	30,36,39	1.47	6 (20%)
5	OMG	L5	1625	5	23,26,27	0.50	0	32,38,41	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	L5	4293	5	18,21,22	1.12	1 (5%)	21,30,33	1.96	4 (19%)
85	A2M	S2	668	85,86	22,25,26	1.29	2 (9%)	30,36,39	1.61	8 (26%)
5	PSU	L5	4312	5	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
85	OMC	S2	462	85	19,22,23	0.54	0	25,31,34	0.71	0
85	A2M	S2	99	85,86	22,25,26	1.16	1 (4%)	30,36,39	1.57	8 (26%)
5	OMU	L5	3925	5	19,22,23	3.32	7 (36%)	25,31,34	1.90	5 (20%)
5	PSU	L5	4403	5	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
85	MA6	S2	1851	85	23,26,27	1.28	2 (8%)	33,38,41	3.42	13 (39%)
85	OMC	S2	1272	85	19,22,23	0.57	0	25,31,34	1.10	2 (8%)
85	PSU	S2	966	85,86	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
85	MA6	S2	1850	85	23,26,27	1.27	2 (8%)	33,38,41	3.34	13 (39%)
5	PSU	L5	3844	5	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
5	OMC	L5	4456	5	19,22,23	0.64	0	25,31,34	0.84	1 (4%)
85	PSU	S2	1081	85	18,21,22	1.04	1 (5%)	21,30,33	1.82	5 (23%)
5	OMC	L5	3841	5	19,22,23	0.56	0	25,31,34	0.69	1 (4%)
5	5MC	L5	4447	5	19,22,23	0.76	0	26,32,35	0.65	0
5	OMC	L5	3808	5	19,22,23	0.64	0	25,31,34	0.78	1 (4%)
5	PSU	L5	3639	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
5	OMG	L5	4370	5	23,26,27	0.48	0	32,38,41	0.49	0
5	PSU	L5	4628	5	18,21,22	1.00	1 (5%)	21,30,33	1.82	4 (19%)
5	PSU	L5	4493	5	18,21,22	1.05	1 (5%)	21,30,33	1.86	3 (14%)
85	4AC	S2	1842	85	21,24,25	0.37	0	28,34,37	0.48	0
5	PSU	L5	3851	5	18,21,22	1.02	1 (5%)	21,30,33	1.86	3 (14%)
5	PSU	L5	4576	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	5 (23%)
5	OMG	L5	4196	5,2	23,26,27	0.49	0	32,38,41	0.45	0
5	OMG	L5	2364	5	23,26,27	0.50	0	32,38,41	0.45	0
85	A2M	S2	468	85	22,25,26	1.18	1 (4%)	30,36,39	1.57	6 (20%)
5	PSU	L5	4636	5	18,21,22	1.10	1 (5%)	21,30,33	2.05	6 (28%)
5	OMG	L5	3792	5	23,26,27	0.49	0	32,38,41	0.53	0
5	A2M	L5	1534	5,86	22,25,26	1.16	2 (9%)	30,36,39	1.52	9 (30%)
5	OMC	L5	2365	5	19,22,23	0.57	0	25,31,34	0.60	0
5	A2M	L5	1524	5	22,25,26	1.22	2 (9%)	30,36,39	1.52	6 (20%)
5	A2M	L5	3825	5	22,25,26	1.13	1 (4%)	30,36,39	1.54	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMC	L5	1340	5	-	1/9/27/28	0/2/2/2
85	A2M	S2	1031	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	1177	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	4579	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3920	5,86	-	0/7/25/26	0/2/2/2
5	PSU	L5	1536	5	-	2/7/25/26	0/2/2/2
5	PSU	L5	4521	5,86	-	0/7/25/26	0/2/2/2
5	OMG	L5	3627	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	4973	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	1288	85	-	2/9/27/28	0/2/2/2
5	PSU	L5	1744	5,86	-	0/7/25/26	0/2/2/2
5	OMG	L5	4499	5	-	1/9/27/28	0/3/3/3
85	PSU	S2	93	85	-	0/7/25/26	0/2/2/2
5	OMU	L5	4306	5	-	0/9/27/28	0/2/2/2
85	4AC	S2	1337	85	-	1/11/29/30	0/2/2/2
5	OMC	L5	2824	5	-	1/9/27/28	0/2/2/2
85	OMG	S2	683	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	651	85	-	0/7/25/26	0/2/2/2
85	OMG	S2	436	85	-	2/9/27/28	0/3/3/3
5	A2M	L5	398	5	-	1/9/27/28	0/3/3/3
5	A2M	L5	4523	5,86	-	0/9/27/28	0/3/3/3
5	PSU	L5	3695	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4500	5	-	3/7/25/26	0/2/2/2
5	PSU	L5	4972	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4471	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	4228	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3867	5	-	3/9/27/28	0/3/3/3
5	UR3	L5	4530	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	1326	85	-	0/9/27/28	0/2/2/2
5	PSU	L5	2632	5	-	0/7/25/26	0/2/2/2
85	OMC	S2	1391	85	-	0/9/27/28	0/2/2/2
85	OMU	S2	116	85	-	0/9/27/28	0/2/2/2
5	PSU	L5	2839	5	-	0/7/25/26	0/2/2/2
85	6MZ	S2	1832	85,86	-	4/12/28/28	0/3/3/3
5	OMC	L5	3701	5	-	6/9/27/28	0/2/2/2
5	OMC	L5	3887	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	1782	5	-	0/7/25/26	0/2/2/2
5	UY1	L5	3818	5	-	2/9/27/28	0/2/2/2
5	PSU	L5	4552	5	-	0/7/25/26	0/2/2/2
85	PSU	S2	406	85	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L5	1860	5	-	0/7/25/26	0/2/2/2
85	A2M	S2	576	85	-	4/9/27/28	0/3/3/3
5	OMC	L5	2861	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	4689	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1677	5	-	3/7/25/26	0/2/2/2
5	A2M	L5	1323	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	1582	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3785	5,86	-	3/9/27/28	0/3/3/3
5	OMC	L5	3869	5	-	1/9/27/28	0/2/2/2
7	OMG	L8	75	7	-	1/9/27/28	0/3/3/3
5	PSU	L5	3884	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1862	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	2351	5,86	-	3/9/27/28	0/2/2/2
5	6MZ	L5	4220	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	2424	5	-	0/9/27/28	0/3/3/3
5	OMC	L5	2804	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	109	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	2815	5	-	2/9/27/28	0/3/3/3
85	PSU	S2	105	85	-	0/7/25/26	0/2/2/2
85	OMU	S2	799	85	-	2/9/27/28	0/2/2/2
85	PSU	S2	801	85	-	2/7/25/26	0/2/2/2
85	OMG	S2	867	85	-	2/9/27/28	0/3/3/3
85	A2M	S2	1383	85	-	3/9/27/28	0/3/3/3
5	OMG	L5	4494	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	400	5	-	1/9/27/28	0/3/3/3
85	A2M	S2	159	85	-	1/9/27/28	0/3/3/3
85	OMG	S2	509	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	686	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	4590	5	-	3/9/27/28	0/3/3/3
85	PSU	S2	1232	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	866	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	5001	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3853	5,86	-	0/7/25/26	0/2/2/2
85	A2M	S2	166	85	-	0/9/27/28	0/3/3/3
5	PSU	L5	4353	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	121	85	-	0/9/27/28	0/2/2/2
85	OMU	S2	1442	85	-	2/9/27/28	0/2/2/2
85	PSU	S2	814	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	4571	5	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OMG	S2	644	85	-	4/9/27/28	0/3/3/3
85	PSU	S2	681	85	-	0/7/25/26	0/2/2/2
5	OMG	L5	4392	5	-	0/9/27/28	0/3/3/3
85	OMU	S2	627	85	-	4/9/27/28	0/2/2/2
5	OMC	L5	2422	5,86	-	2/9/27/28	0/2/2/2
5	OMC	L5	4536	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4673	5,86	-	0/7/25/26	0/2/2/2
85	OMC	S2	1703	85	-	1/9/27/28	0/2/2/2
85	OMC	S2	517	85	-	2/9/27/28	0/2/2/2
5	PSU	L5	1781	5	-	1/7/25/26	0/2/2/2
5	PSU	L5	4457	5	-	0/7/25/26	0/2/2/2
85	PSU	S2	1056	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	3718	5	-	1/9/27/28	0/3/3/3
5	OMG	L5	2876	5	-	1/9/27/28	0/3/3/3
5	A2M	L5	3830	5	-	0/9/27/28	0/3/3/3
85	PSU	S2	1004	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	1367	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	2401	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	4442	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	354	85	-	0/9/27/28	0/2/2/2
85	A2M	S2	27	85	-	1/9/27/28	0/3/3/3
85	PSU	S2	863	85	-	0/7/25/26	0/2/2/2
5	OMU	L5	2837	5	-	0/9/27/28	0/2/2/2
5	OMG	L5	1316	5	-	0/9/27/28	0/3/3/3
5	OMU	L5	4227	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	1174	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	1244	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	4431	5	-	0/7/25/26	0/2/2/2
85	PSU	S2	1045	85	-	2/7/25/26	0/2/2/2
5	OMG	L5	3744	5	-	0/9/27/28	0/3/3/3
85	PSU	S2	1046	85	-	0/7/25/26	0/2/2/2
85	OMC	S2	174	85	-	1/9/27/28	0/2/2/2
85	OMU	S2	172	85	-	0/9/27/28	0/2/2/2
5	A2M	L5	2787	5	-	6/9/27/28	0/3/3/3
85	OMG	S2	1490	85	-	1/9/27/28	0/3/3/3
5	PSU	L5	3637	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4618	5	-	2/9/27/28	0/3/3/3
85	PSU	S2	649	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	5010	5	-	0/7/25/26	0/2/2/2
85	OMG	S2	601	85	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PSU	L8	69	7	-	0/7/25/26	0/2/2/2
5	OMG	L5	4623	5	-	0/9/27/28	0/3/3/3
85	B8N	S2	1248	85	-	5/16/34/35	0/2/2/2
5	1MA	L5	1322	5,86	-	2/7/25/26	0/3/3/3
5	PSU	L5	4299	5	-	0/7/25/26	0/2/2/2
5	OMU	L5	4498	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4532	5	-	0/7/25/26	0/2/2/2
7	PSU	L8	55	7	-	0/7/25/26	0/2/2/2
5	PSU	L5	1792	5	-	0/7/25/26	0/2/2/2
5	5MC	L5	3782	5,86	-	1/7/25/26	0/2/2/2
5	OMG	L5	3899	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	3822	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	1871	5,86	-	0/9/27/28	0/3/3/3
5	A2M	L5	1326	5	-	3/9/27/28	0/3/3/3
5	PSU	L5	4361	5	-	0/7/25/26	0/2/2/2
85	OMG	S2	1328	85	-	1/9/27/28	0/3/3/3
5	A2M	L5	2363	5,86	-	0/9/27/28	0/3/3/3
5	PSU	L5	1683	5	-	0/7/25/26	0/2/2/2
85	G7M	S2	1639	85,2	-	0/7/25/26	0/3/3/3
5	OMG	L5	1522	5	-	0/9/27/28	0/3/3/3
3	SEP	CF	163	3	-	6/6/8/10	-
5	OMU	L5	4620	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4296	5	-	2/7/25/26	0/2/2/2
5	OMG	L5	4637	5	-	3/9/27/28	0/3/3/3
85	OMU	S2	428	85	-	6/9/27/28	0/2/2/2
85	A2M	S2	484	85	-	0/9/27/28	0/3/3/3
5	OMG	L5	1625	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	4293	5	-	0/7/25/26	0/2/2/2
85	A2M	S2	668	85,86	-	2/9/27/28	0/3/3/3
5	PSU	L5	4312	5	-	0/7/25/26	0/2/2/2
85	OMC	S2	462	85	-	0/9/27/28	0/2/2/2
85	A2M	S2	99	85,86	-	3/9/27/28	0/3/3/3
5	OMU	L5	3925	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4403	5	-	0/7/25/26	0/2/2/2
85	MA6	S2	1851	85	-	1/11/29/30	0/3/3/3
85	OMC	S2	1272	85	-	5/9/27/28	0/2/2/2
85	PSU	S2	966	85,86	-	0/7/25/26	0/2/2/2
85	MA6	S2	1850	85	-	0/11/29/30	0/3/3/3
5	PSU	L5	3844	5	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMC	L5	4456	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	1081	85	-	1/7/25/26	0/2/2/2
5	OMC	L5	3841	5	-	1/9/27/28	0/2/2/2
5	5MC	L5	4447	5	-	4/7/25/26	0/2/2/2
5	OMC	L5	3808	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	3639	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4370	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	4628	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4493	5	-	0/7/25/26	0/2/2/2
85	4AC	S2	1842	85	-	0/11/29/30	0/2/2/2
5	PSU	L5	3851	5	-	1/7/25/26	0/2/2/2
5	PSU	L5	4576	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4196	5,2	-	1/9/27/28	0/3/3/3
5	OMG	L5	2364	5	-	1/9/27/28	0/3/3/3
85	A2M	S2	468	85	-	0/9/27/28	0/3/3/3
5	PSU	L5	4636	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	3792	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	1534	5,86	-	1/9/27/28	0/3/3/3
5	OMC	L5	2365	5	-	0/9/27/28	0/2/2/2
5	A2M	L5	1524	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3825	5	-	0/9/27/28	0/3/3/3

The worst 5 of 271 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	3818	UY1	C6-C5	12.73	1.49	1.35
85	S2	1832	6MZ	C6-N6	12.64	1.48	1.34
5	L5	4220	6MZ	C6-N6	12.38	1.48	1.34
5	L5	3818	UY1	C2-N1	11.79	1.52	1.36
85	S2	1442	OMU	C2-N1	8.47	1.51	1.38

The worst 5 of 672 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1851	MA6	N1-C6-N6	-12.17	102.03	116.86
85	S2	1850	MA6	N1-C6-N6	-11.70	102.60	116.86
85	S2	1851	MA6	C5-C6-N6	8.11	138.17	125.33
85	S2	1850	MA6	C5-C6-N6	7.86	137.77	125.33
85	S2	1639	G7M	C1'-N9-C4	7.66	149.10	126.49

There are no chirality outliers.

5 of 162 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CF	163	SEP	N-CA-CB-OG
3	CF	163	SEP	C-CA-CB-OG
3	CF	163	SEP	CA-CB-OG-P
3	CF	163	SEP	CB-OG-P-O2P
3	CF	163	SEP	CB-OG-P-O3P

There are no ring outliers.

75 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	1340	OMC	2	0
85	S2	1031	A2M	1	0
85	S2	1177	PSU	1	0
5	L5	4579	PSU	2	0
5	L5	3627	OMG	1	0
85	S2	1288	OMU	1	0
5	L5	4306	OMU	1	0
85	S2	1337	4AC	4	0
5	L5	2824	OMC	1	0
85	S2	436	OMG	1	0
5	L5	4523	A2M	2	0
5	L5	4500	PSU	1	0
5	L5	3867	A2M	3	0
85	S2	1391	OMC	1	0
85	S2	1832	6MZ	1	0
5	L5	3701	OMC	1	0
85	S2	576	A2M	2	0
5	L5	2861	OMC	1	0
5	L5	4689	PSU	1	0
5	L5	1677	PSU	1	0
5	L5	3785	A2M	1	0
7	L8	75	OMG	2	0
5	L5	3884	PSU	1	0
5	L5	2351	OMC	1	0
5	L5	4220	6MZ	1	0
5	L5	2424	OMG	1	0
5	L5	2804	OMC	2	0
5	L5	2815	A2M	1	0
85	S2	867	OMG	2	0
85	S2	1383	A2M	1	0
5	L5	400	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	S2	159	A2M	2	0
85	S2	509	OMG	3	0
85	S2	686	PSU	1	0
5	L5	4590	A2M	1	0
85	S2	866	PSU	2	0
5	L5	5001	PSU	1	0
85	S2	166	A2M	2	0
85	S2	121	OMU	1	0
5	L5	4571	A2M	2	0
85	S2	681	PSU	1	0
5	L5	4536	OMC	1	0
85	S2	517	OMC	1	0
5	L5	4457	PSU	1	0
5	L5	3718	A2M	4	0
5	L5	2876	OMG	1	0
85	S2	27	A2M	1	0
85	S2	863	PSU	1	0
85	S2	1174	PSU	2	0
85	S2	1244	PSU	1	0
5	L5	4431	PSU	1	0
5	L5	2787	A2M	1	0
5	L5	4618	OMG	1	0
85	S2	649	PSU	2	0
85	S2	601	OMG	1	0
5	L5	3822	PSU	2	0
5	L5	1326	A2M	4	0
5	L5	2363	A2M	1	0
5	L5	1683	PSU	2	0
3	CF	163	SEP	1	0
5	L5	4620	OMU	3	0
5	L5	4637	OMG	1	0
85	S2	484	A2M	1	0
85	S2	462	OMC	1	0
85	S2	99	A2M	1	0
5	L5	3925	OMU	1	0
85	S2	1272	OMC	1	0
85	S2	1850	MA6	2	0
5	L5	4456	OMC	1	0
5	L5	3841	OMC	1	0
85	S2	1842	4AC	1	0
5	L5	2364	OMG	1	0
85	S2	468	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	1534	A2M	2	0
5	L5	3825	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.92	0
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.86	0
88	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.68	0
88	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.88	0
88	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.88	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.91	0
88	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
87	SPM	L5	5267	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPD	L5	5282	-	9,9,9	0.34	0	8,8,8	0.84	0
88	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.95	0
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	0.98	0
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.87	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPM	L5	5264	-	-	2/11/11/11	-
88	SPD	L5	5289	-	-	2/7/7/7	-
88	SPD	L5	5290	-	-	2/7/7/7	-
88	SPD	L5	5286	-	-	3/7/7/7	-
88	SPD	L5	5285	-	-	1/7/7/7	-
88	SPD	LN	301	-	-	1/7/7/7	-
87	SPM	L5	5291	-	-	3/11/11/11	-
87	SPM	L5	5292	-	-	5/11/11/11	-
88	SPD	L5	5287	-	-	1/7/7/7	-
87	SPM	L5	5263	-	-	6/11/11/11	-
87	SPM	L5	5267	-	-	4/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5261	-	-	0/7/7/7	-
88	SPD	L5	5283	-	-	4/7/7/7	-
87	SPM	L5	5288	-	-	5/11/11/11	-
88	SPD	L5	5284	-	-	4/7/7/7	-
87	SPM	L5	5258	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5264	SPM	N5-C6-C7-C8
87	L5	5291	SPM	C7-C8-C9-N10
88	L5	5286	SPD	C3-C4-C5-N6
87	L5	5291	SPM	N5-C6-C7-C8
87	L5	5292	SPM	N10-C11-C12-C13

There are no ring outliers.

5 monomers are involved in 7 short contacts:

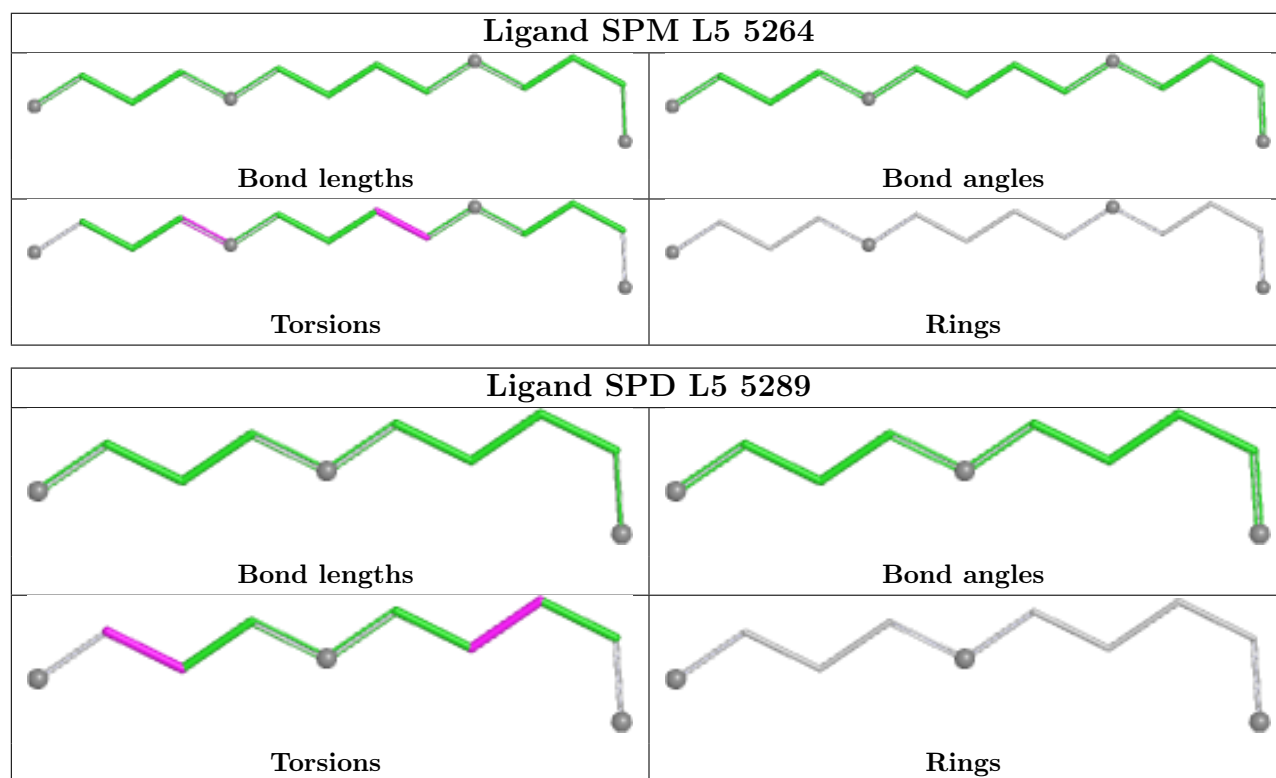
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5290	SPD	1	0
88	L5	5285	SPD	1	0
87	L5	5291	SPM	2	0

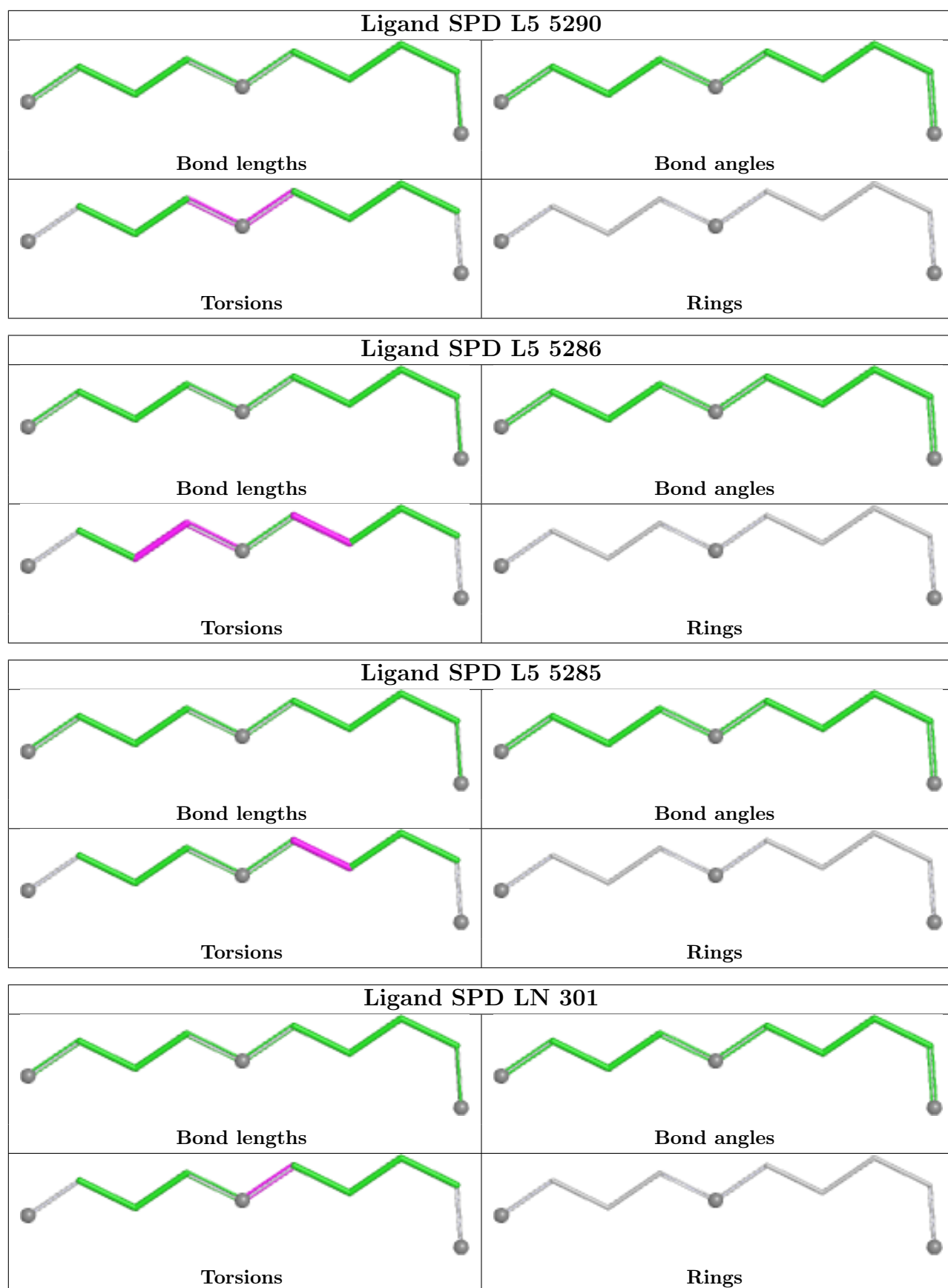
Continued on next page...

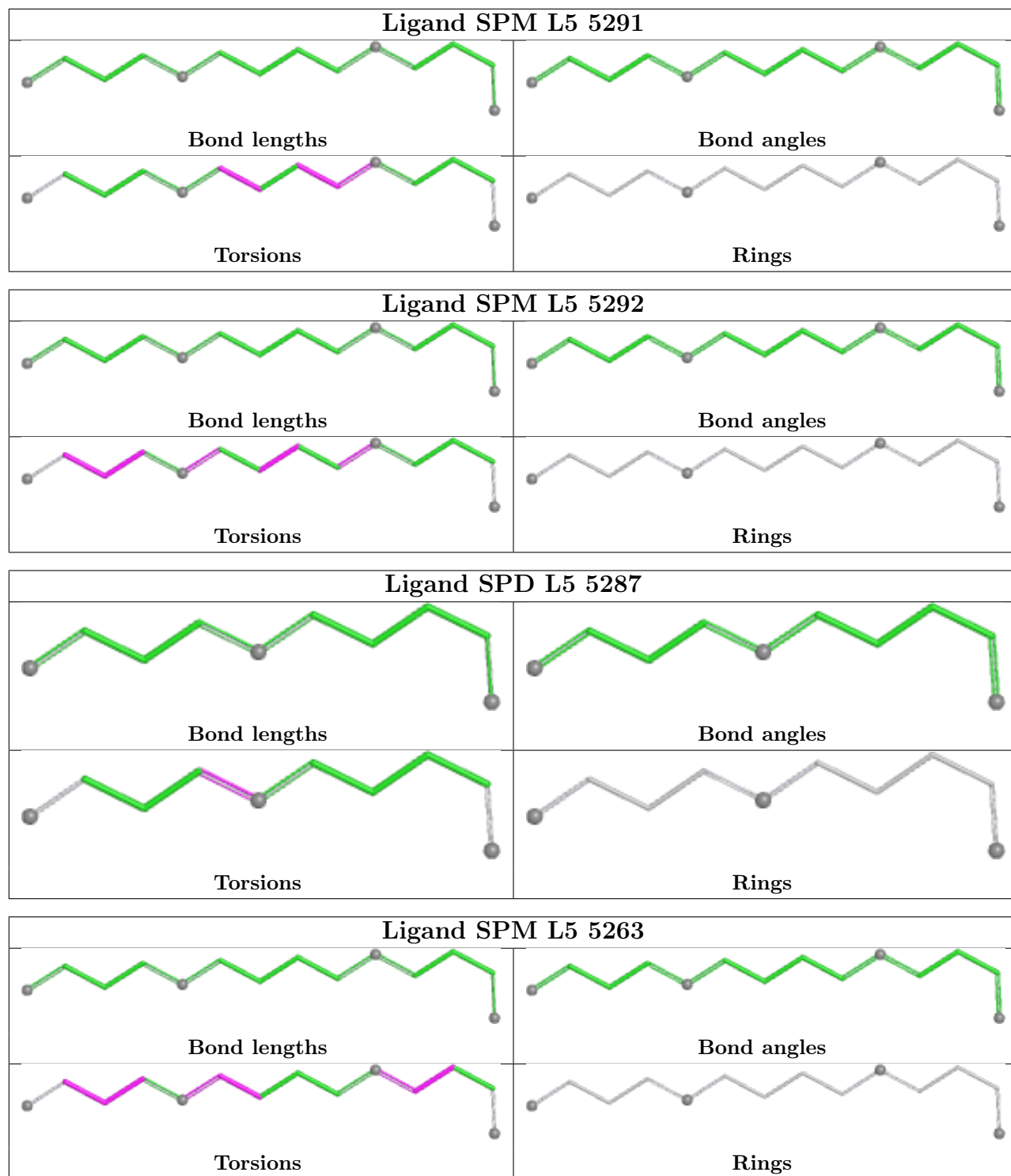
Continued from previous page...

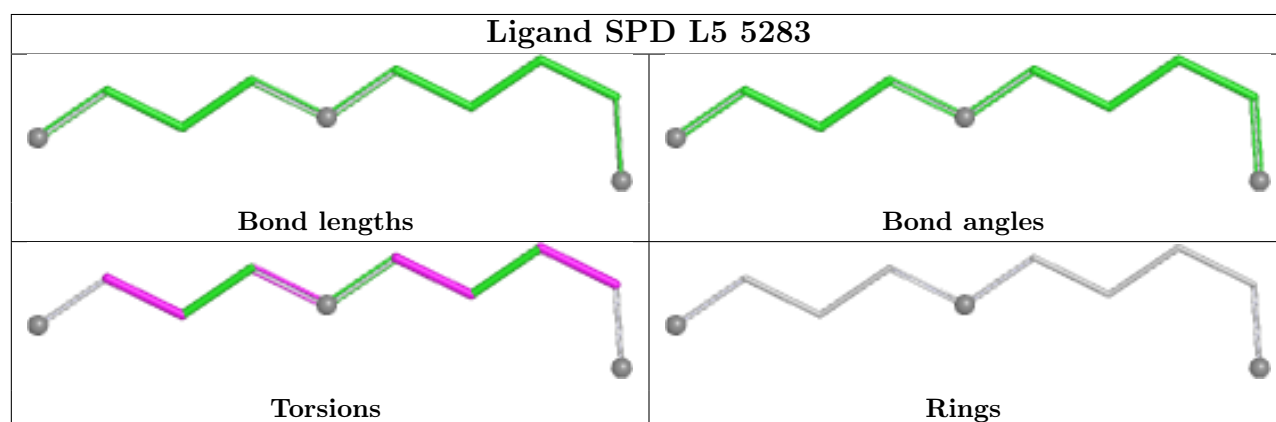
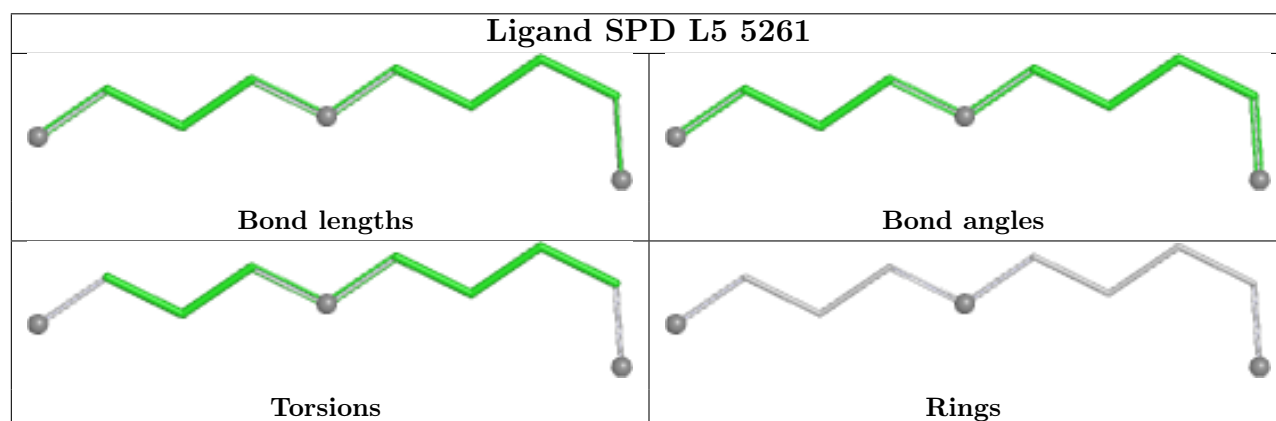
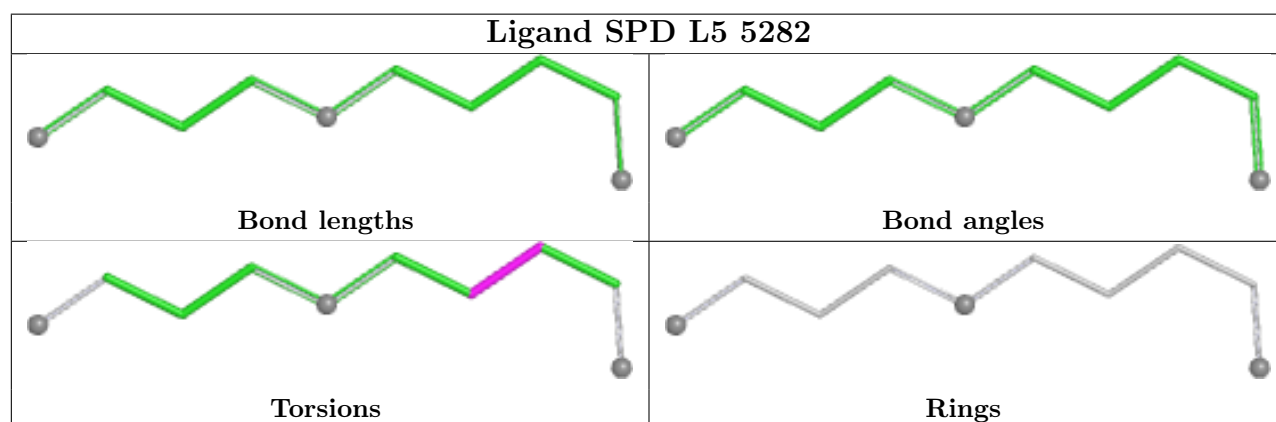
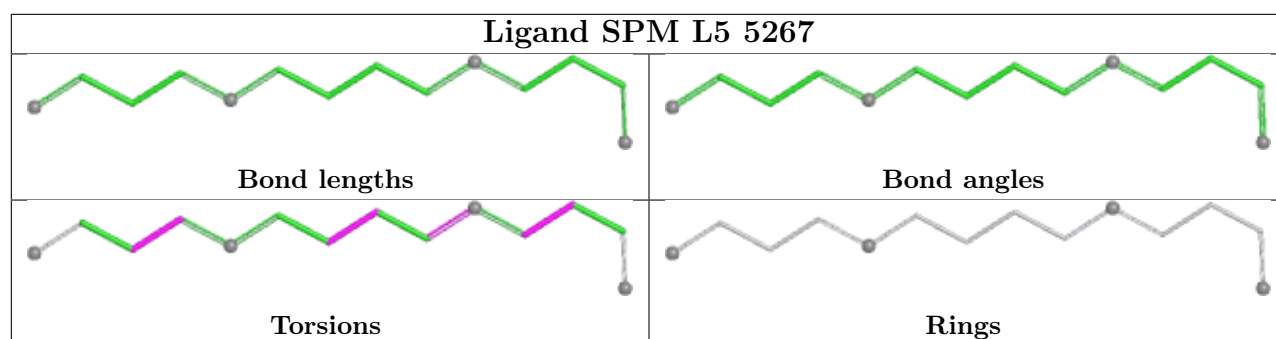
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5292	SPM	2	0
88	L5	5261	SPD	1	0

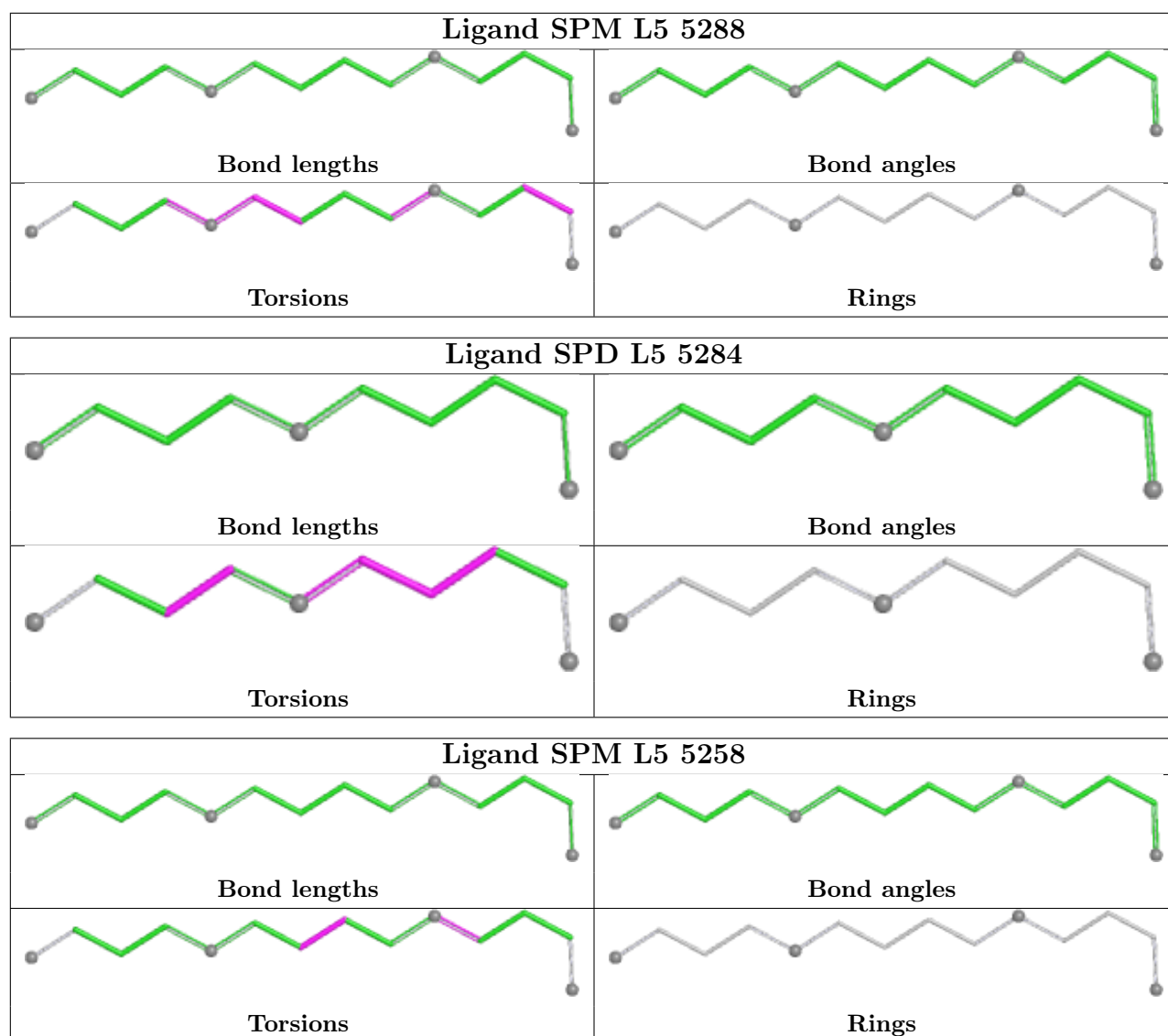
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L5	10
85	S2	5
2	Pt	1
4	AT	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.79
1	L5	1706:A	O3'	1716:G	P	21.22
1	L5	2910:G	O3'	3584:C	P	21.08
1	L5	760:G	O3'	903:C	P	16.76
1	L5	519:C	O3'	642:G	P	15.26

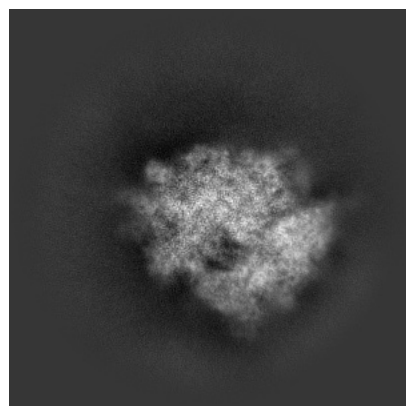
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71333. These allow visual inspection of the internal detail of the map and identification of artifacts.

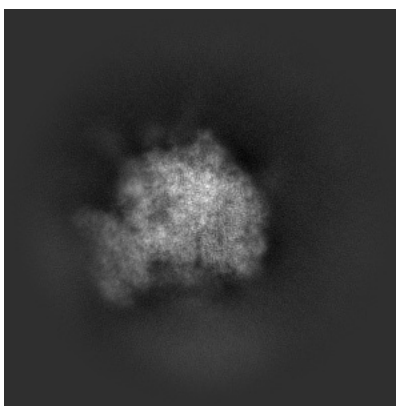
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

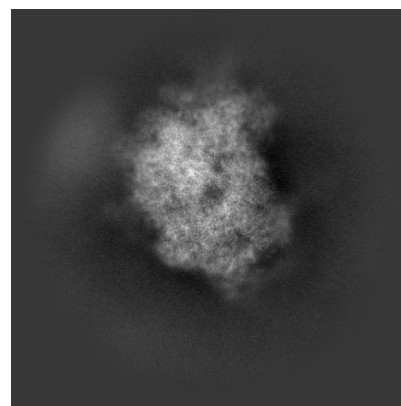
6.1.1 Primary map



X

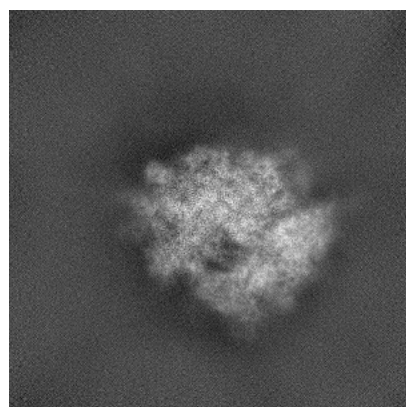


Y

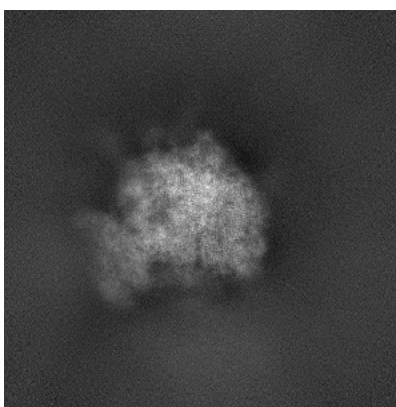


Z

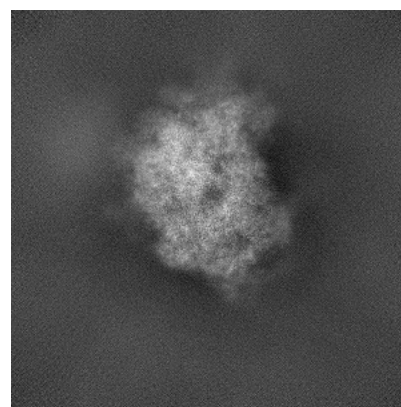
6.1.2 Raw map



X



Y

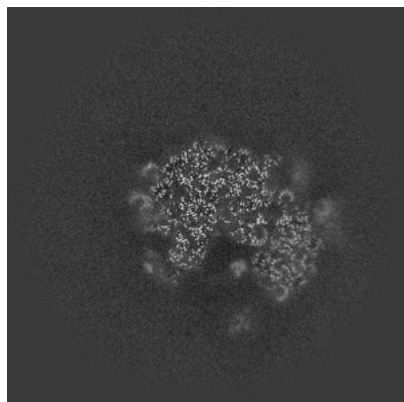


Z

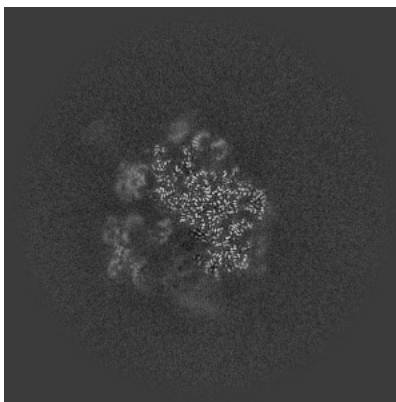
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

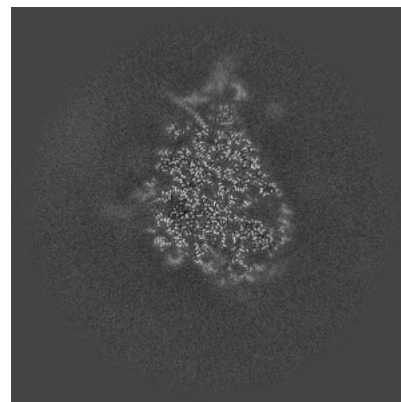
6.2.1 Primary map



X Index: 256

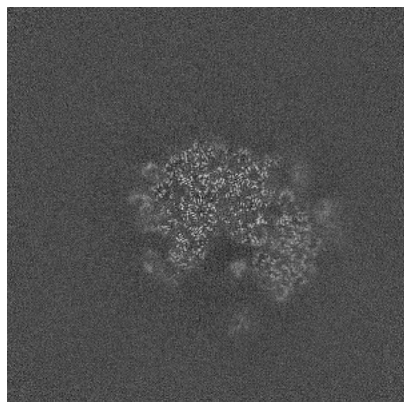


Y Index: 256

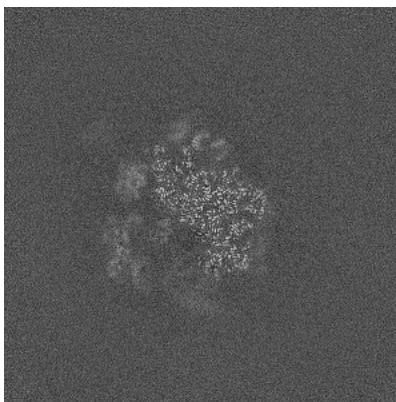


Z Index: 256

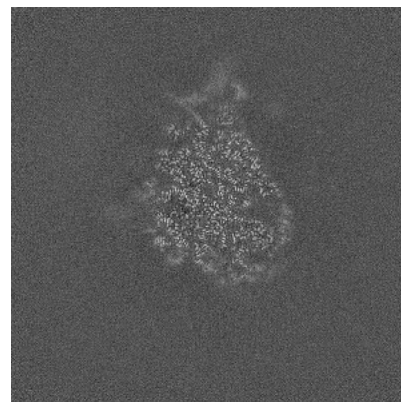
6.2.2 Raw map



X Index: 256



Y Index: 256

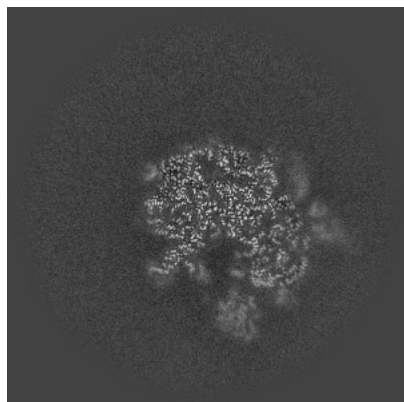


Z Index: 256

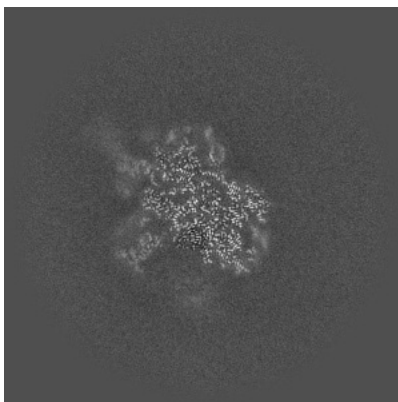
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

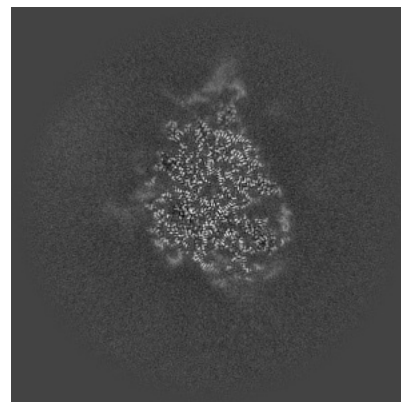
6.3.1 Primary map



X Index: 244

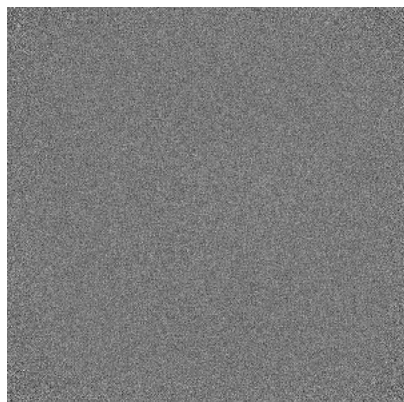


Y Index: 243

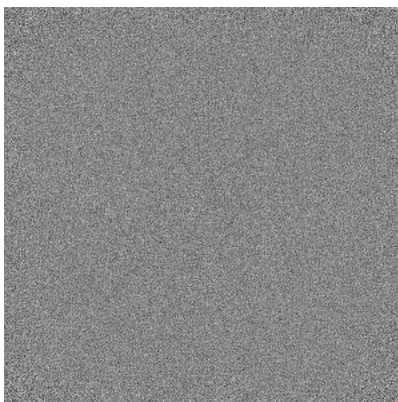


Z Index: 258

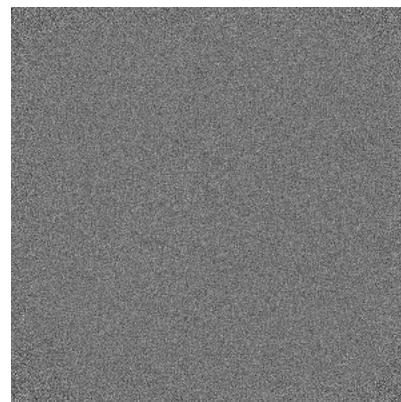
6.3.2 Raw map



X Index: 0



Y Index: 0

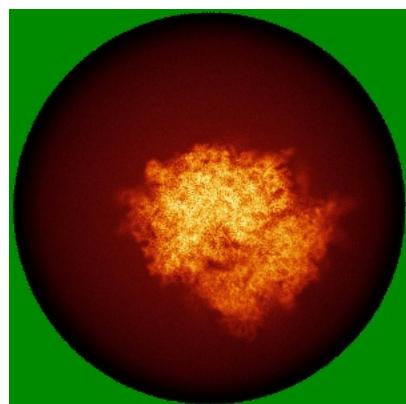


Z Index: 0

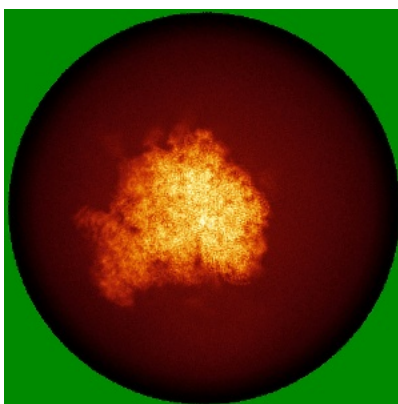
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

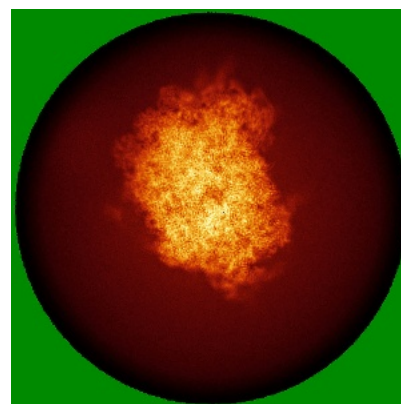
6.4.1 Primary map



X

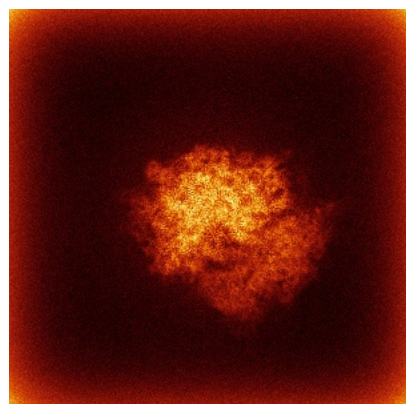


Y

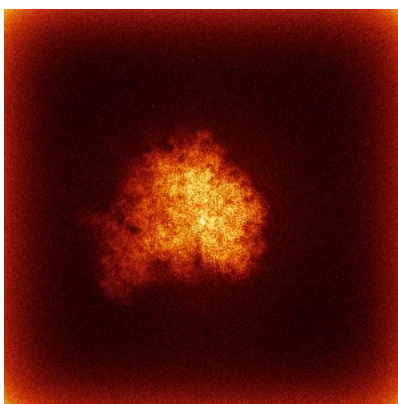


Z

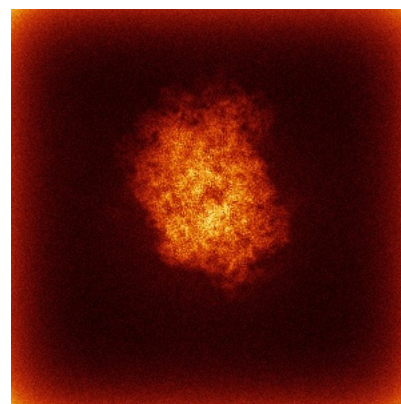
6.4.2 Raw map



X



Y

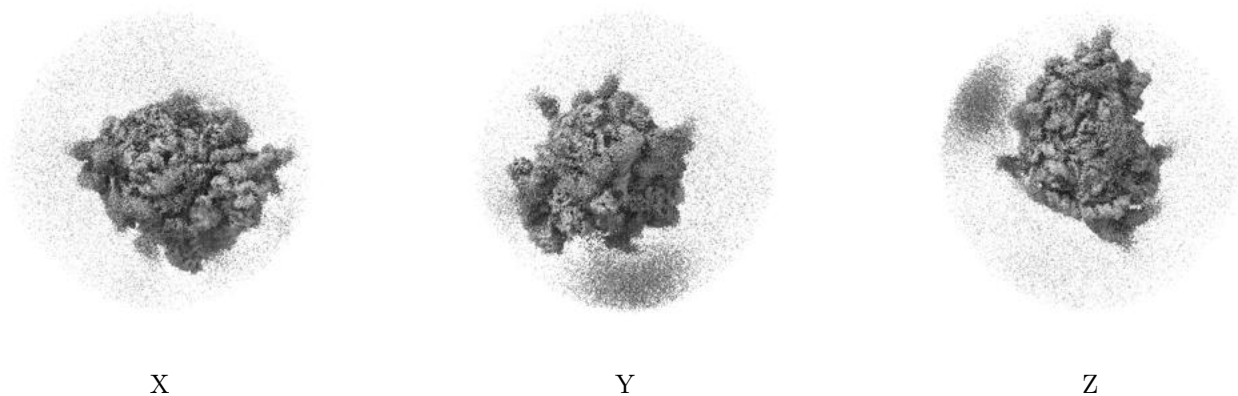


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

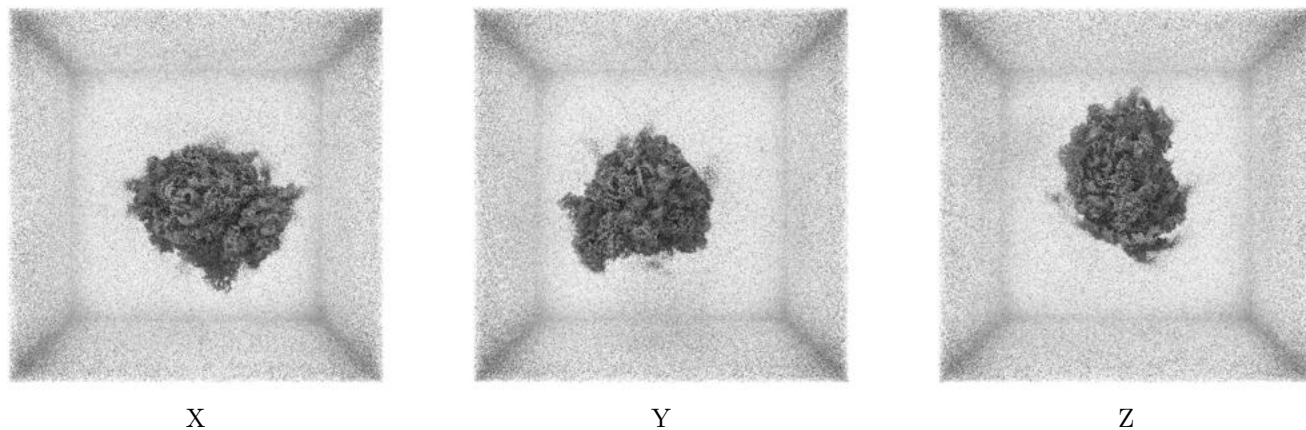
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

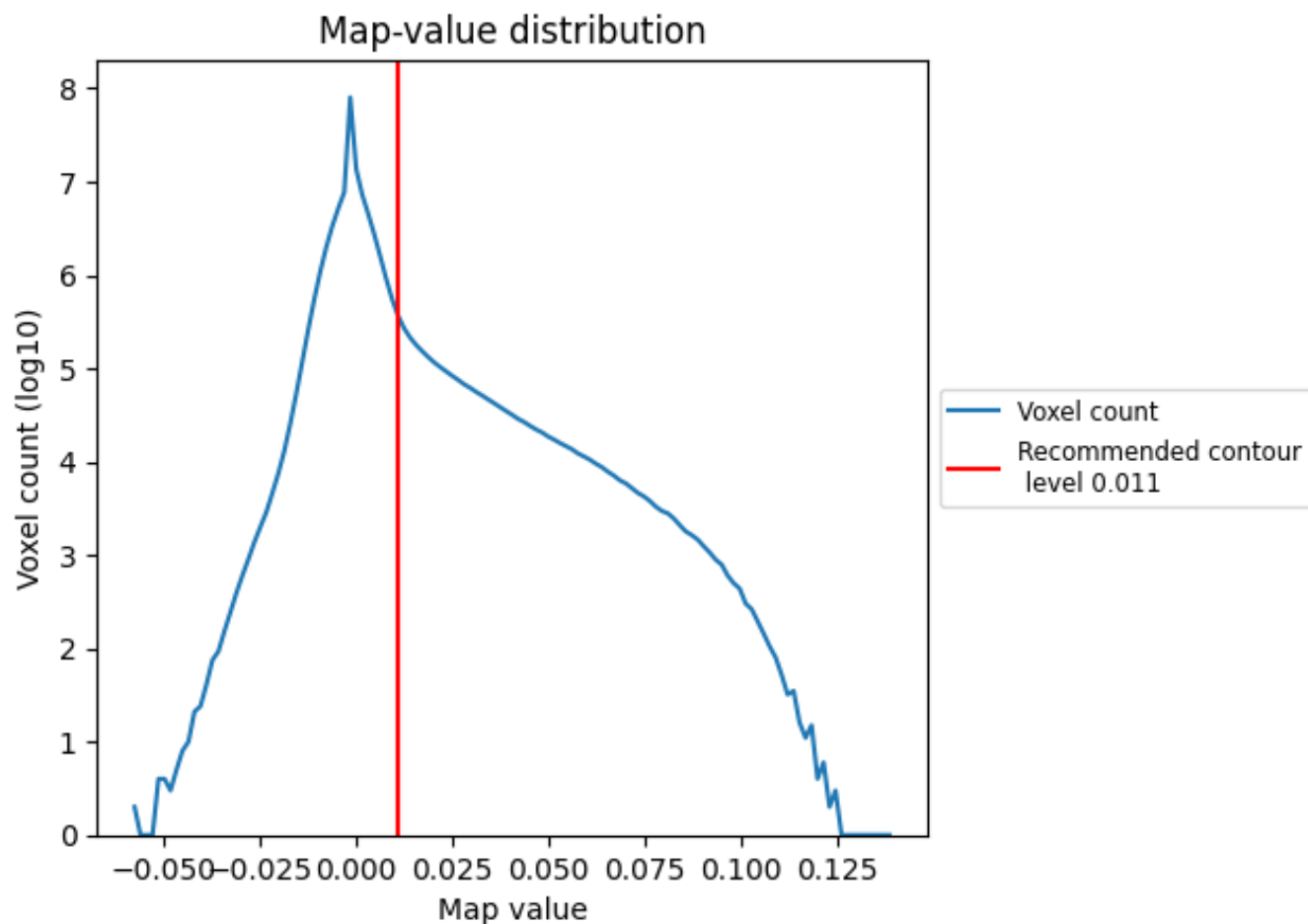
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

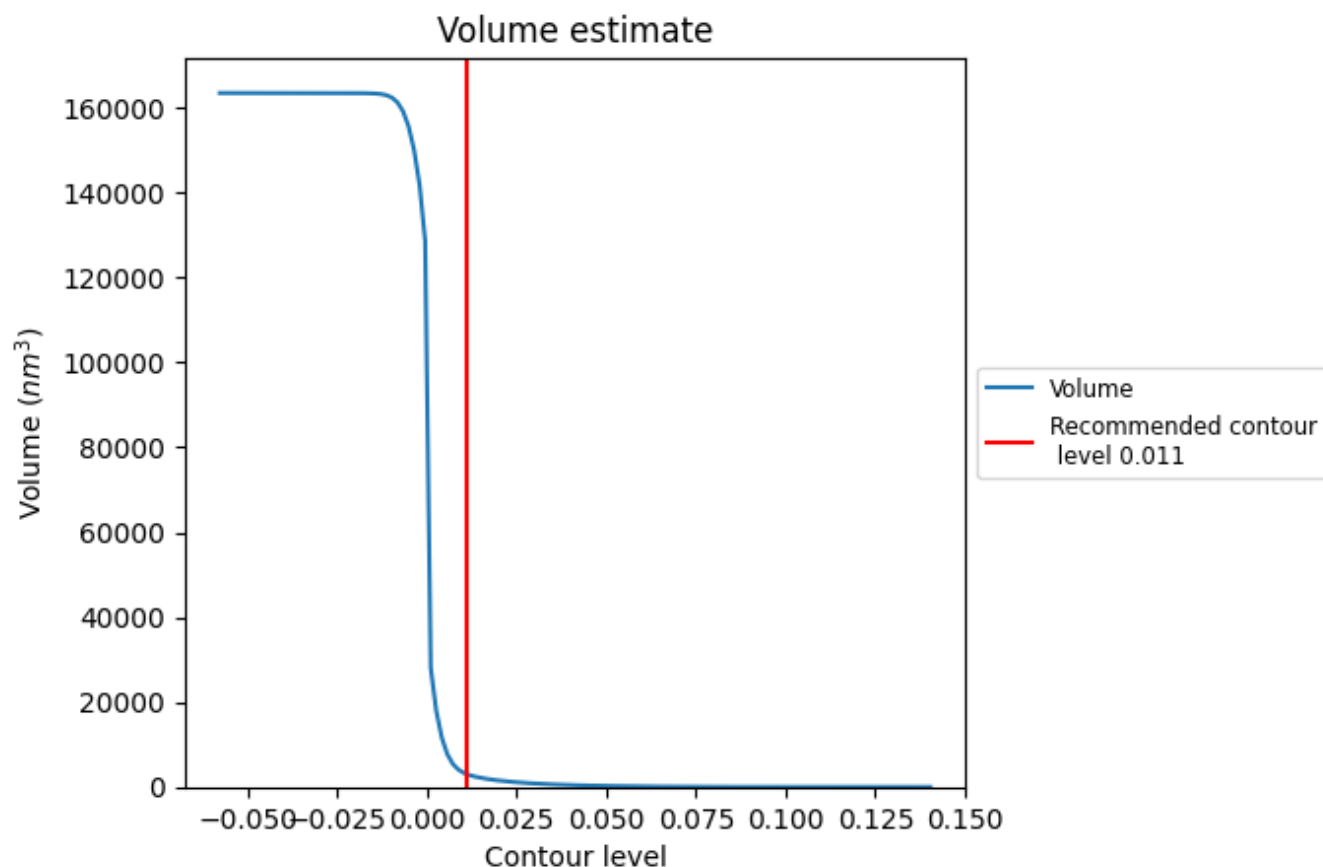
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

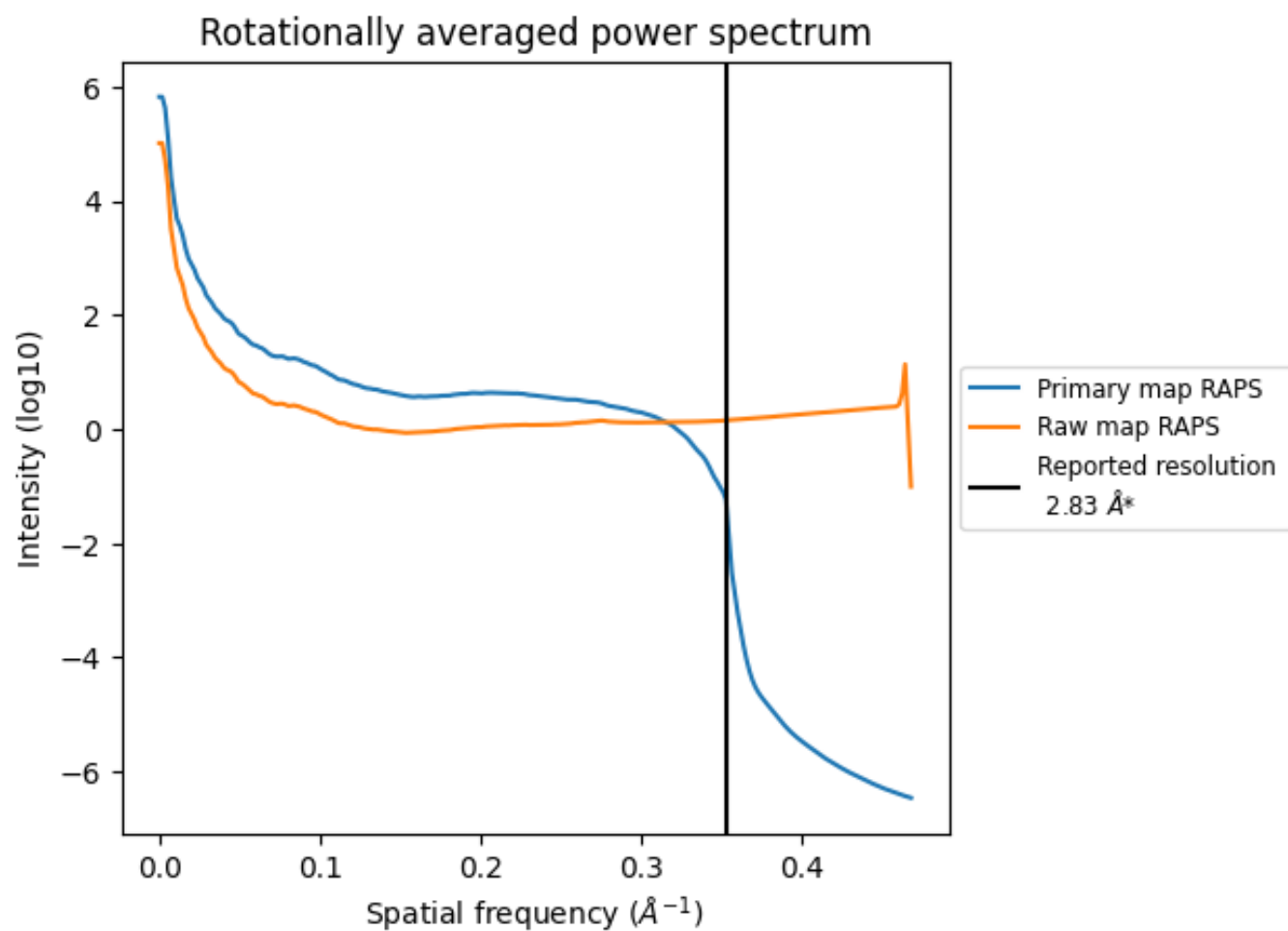
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3087 nm^3 ; this corresponds to an approximate mass of 2789 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

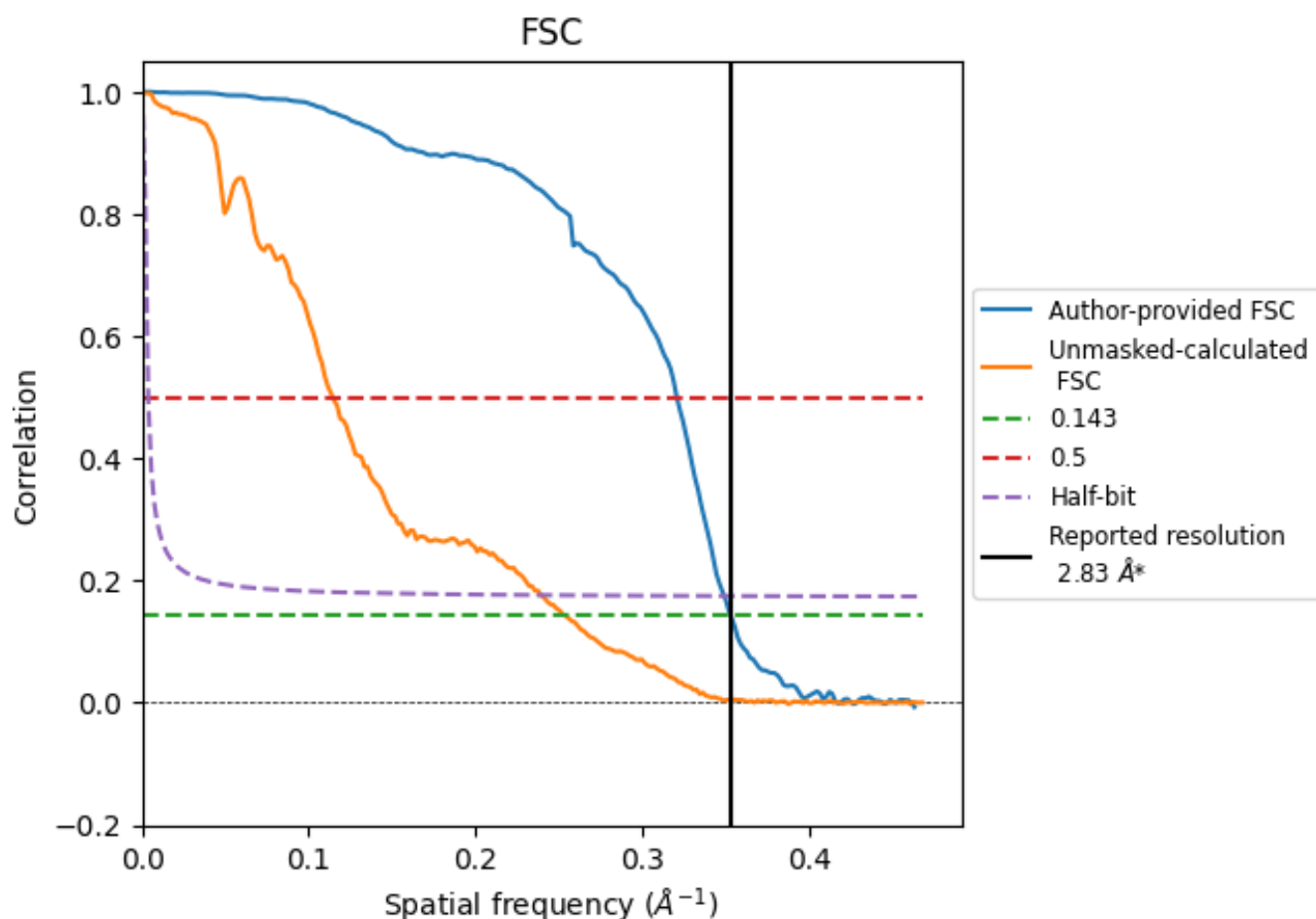


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

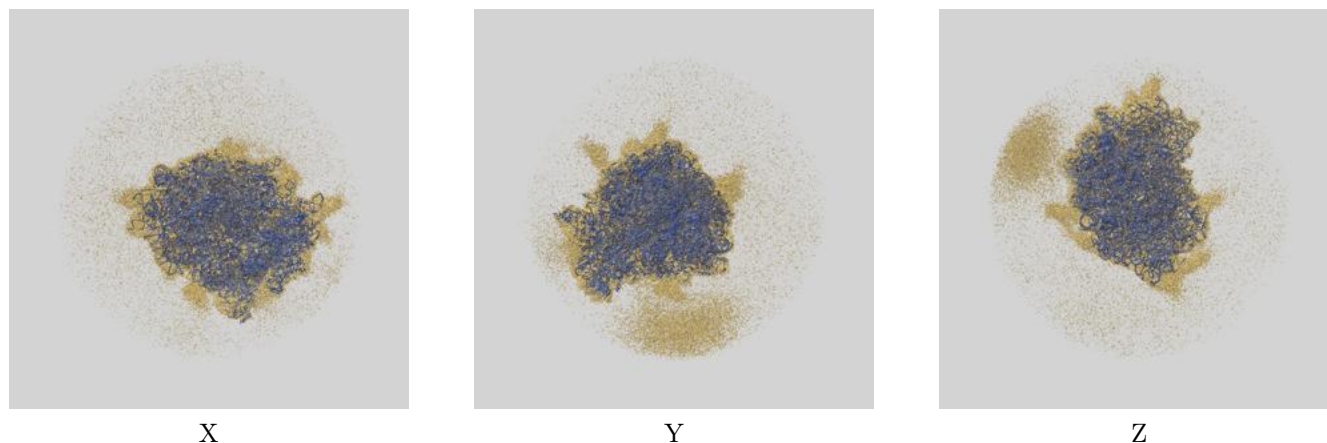
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.12	2.86
Unmasked-calculated*	3.94	8.74	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

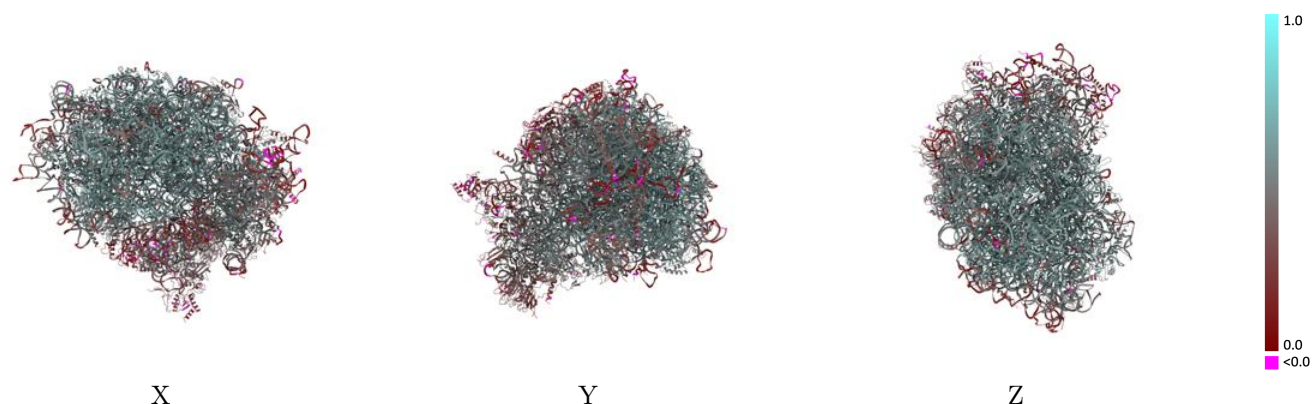
This section contains information regarding the fit between EMDB map EMD-71333 and PDB model 9P76. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



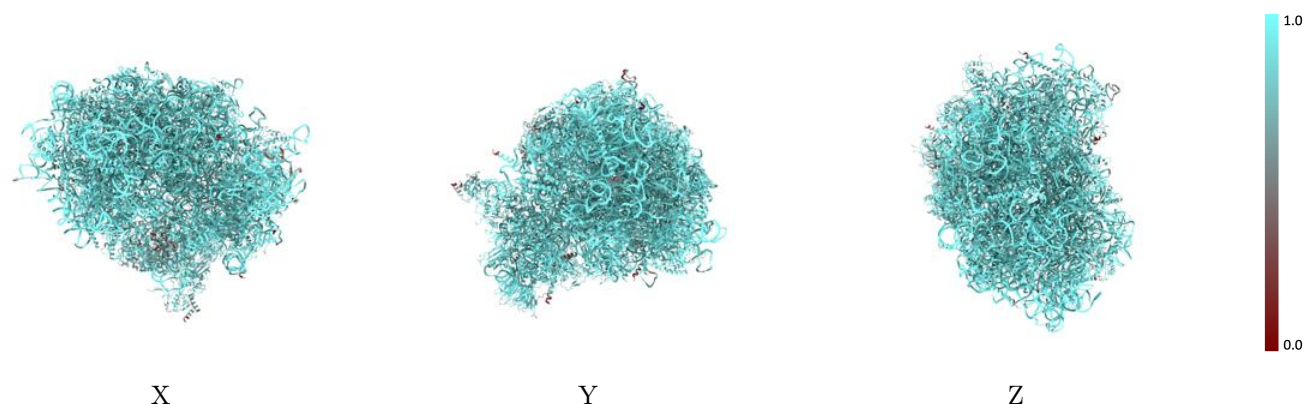
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



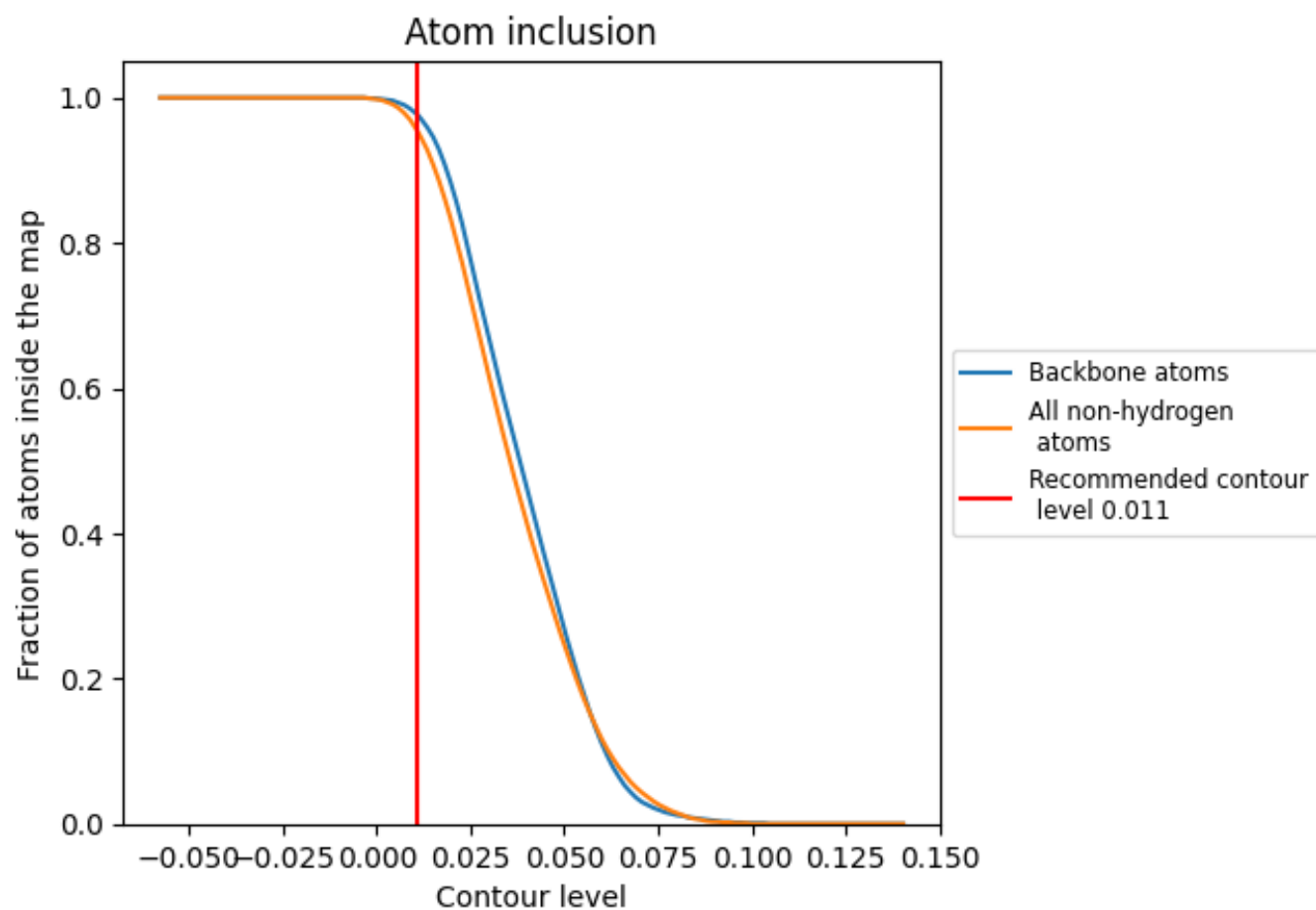
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4970
AT	 0.9730	 0.2490
CF	 0.9150	 0.2820
CI	 0.7280	 0.4080
L5	 0.9810	 0.5300
L7	 0.9970	 0.5750
L8	 0.9880	 0.5580
LA	 0.9800	 0.5910
LB	 0.9500	 0.5700
LC	 0.9570	 0.5720
LD	 0.9520	 0.5310
LE	 0.9030	 0.5020
LF	 0.9730	 0.5730
LG	 0.9080	 0.5060
LH	 0.9560	 0.5580
LI	 0.9480	 0.5660
LJ	 0.9310	 0.5030
LL	 0.9210	 0.5420
LM	 0.9650	 0.5600
LN	 0.9910	 0.6100
LO	 0.9630	 0.5730
LP	 0.9650	 0.5840
LQ	 0.9660	 0.5950
LR	 0.9110	 0.5140
LS	 0.9710	 0.5920
LT	 0.9450	 0.5530
LU	 0.9390	 0.4820
LV	 0.9550	 0.5770
LW	 0.8720	 0.3930
LX	 0.9380	 0.5510
LY	 0.9580	 0.5570
LZ	 0.9730	 0.5440
La	 0.9740	 0.5940
Lb	 0.9050	 0.4940
Lc	 0.9480	 0.5320



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Chain	Atom inclusion	Q-score
Ld	 0.9350	 0.5520
Le	 0.9750	 0.5900
Lf	 0.9830	 0.6020
Lg	 0.9620	 0.5680
Lh	 0.9400	 0.5480
Li	 0.9520	 0.5410
Lj	 0.9790	 0.5970
Lk	 0.8900	 0.4930
Ll	 0.9690	 0.5790
Lm	 0.9380	 0.5730
Ln	 0.9570	 0.5540
Lo	 0.8180	 0.5720
Lp	 0.9420	 0.5640
Lr	 0.9640	 0.5750
Ls	 0.6340	 0.2010
Lt	 0.6340	 0.1710
Pt	 0.9190	 0.4450
S2	 0.9840	 0.4680
SA	 0.9180	 0.4560
SB	 0.9170	 0.4900
SC	 0.9540	 0.4920
SD	 0.9020	 0.3800
SE	 0.9450	 0.4600
SF	 0.7670	 0.4200
SG	 0.8820	 0.3620
SH	 0.8830	 0.3780
SI	 0.9140	 0.4770
SJ	 0.9270	 0.4520
SK	 0.9120	 0.3390
SL	 0.9020	 0.5050
SM	 0.6910	 0.1680
SN	 0.9430	 0.5200
SO	 0.8930	 0.5140
SP	 0.8520	 0.3570
SQ	 0.9190	 0.4040
SR	 0.8860	 0.3890
SS	 0.8840	 0.3950
ST	 0.9310	 0.3990
SU	 0.9040	 0.3540
SV	 0.9500	 0.4620
SW	 0.9630	 0.5230
SX	 0.9260	 0.5080

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Chain	Atom inclusion	Q-score
SY	 0.8980	 0.3880
SZ	 0.6450	 0.3720
Sa	 0.9480	 0.5120
Sb	 0.9220	 0.4580
Sc	 0.8020	 0.3950
Sd	 0.9550	 0.4510
Se	 0.8290	 0.3980
Sf	 0.7860	 0.2150
Sg	 0.8850	 0.3180